Name	Name of Journal/Conferenc	Title of the paper	Abstract	Impact/Significance	Page Link	Publication Yea
Deepthi Padmanabhan, Adil Lateef, Purushothaman Natarajan, Senthilkumar Palanisamy	Molecular Biology Reports	De novo transcriptome analysis of Justicia adhatoda reveals candidate genes involved in major biosynthetic pathway	Justicia adhatoda is an important medicinal plant traditionally used in the Indian system of medicine and the absence of molecular-level studies in this plant hinders its wide use, hence the study was aimed to analyse the genes involved in its various pathways. The RNA isolated was subjected to Illumina sequencing. De novo assembly was performed using TRINITY software which produced 171,064 transcripts with 55,528 genes and N50 value of 2065 bp, followed by annotation of unigenes against NCBI, KEGG and Gene ontology databases resulted in 105,572 annotated unigenes and 40,288 non-annotated unigenes. A total of 5980 unigenes were mapped to 144 biochemical pathways, including the metabolism and biosynthesis pathways. The pathway analysis revealed the major transcripts involved in the tryptophan biosynthesis with TPM values of 6.0903, 33.6854, 11.527, 1.6959, and 8.1662 for Anthranilate synthase alpha, Anthranilate synthase beta, Arogenate/Prephenate dehydratase, Chorismate synthase and Chorismate mutase, respectively. The qRT-PCR validation of the key enzymes showed up-regulation in mid mature leaf when compared to root and young leaf tissue. A total of 16,154 SSRs were identified from the leaf transcriptome of J. adhatoda ,which could be helpful in molecular breeding. The study aimed at identifying transcripts involved in the tryptophan biosynthesis pathway for its medicinal properties, as it acts as a precursor to the acridone alkaloid biosynthesis with major key enzymes and their validation. This is the first study that reports transcriptome assembly and annotation of J. adhatoda plant.	This study sheds light on the molecular pathways of Justicia adhatoda, an important medicinal plant in Indian traditional medicine. By identifying key genes involved in tryptophan biosynthesis, it lays the foundation for understanding its medicinal properties and potential applications. Additionally, the discovery of SSR markers offers prospects for molecular breeding, enhancing its cultivation and therapeutic potential.	https://link.springer.com/article/10.1007/s11033-022-07784-5	2022
Deepthi Padmanabhan, Purushothaman Natarajan, Senthilkumar Palanisamy	Genes	Integrated Metabolite and Transcriptome Profiling-Mediated Gene Mining of Sida cordifolia Reveals Medicinally Important Genes	Sida cordifolia is a medicinal shrub that is conventionally used in the Indian system of medicine;however, the genes contributing to its medicinal properties have been minimally explored, thus limiting its application. High-throughputsequencing and Liquid Chromatography with tandem mass spectrometry(LC-MS/MS) technologies were applied to unravel the medicinally important bioactive compounds. As a result, transcriptomic sequencing generated more than 12 GB of clean data, and 187,215 transcripts were obtained by de novoassembly. These transcripts were broadly classified into 20 classes, based on the gene ontology classification, and 6551 unigenes were annotated using Kyoto Encyclopedia of Genes and Genomes (KEGG) database with more than 142 unigenes involved in the biosynthesis of secondary metabolites. LC-MS/MS analysis of three tissues of Sida cordifolia revealed that acacetin and procyanidin are some important metabolites identified thatcontribute to its medicinal value. Several key enzymes witha crucial role in phenylpropanoid and flavonoid biosynthetic pathways were identified, especially phenylalanine ammonia lyase, which might be an important rate-limiting enzyme. Real-Time Quantitative Reverse Transcription Polymerase chain reaction (qRT-PCR) analysis revealed enzymes, such as Phenylalanine ammonia lyase (PAL), Cinnamyl alcohol dehydrogenase 1 (CAD), Cinnamoyl-CoA reductase 1 (CF1) and Trans cinnamate 4-monooxygenase(TCM), which were predominantly expressed in root compared to leaf and stem tissue. The study provides a speculative insight for the screening of active metabolites and metabolic engineering in Sida cordifolia.	This groundbreaking study on Sida cordifolia unlocks its medicinal potential by identifying key genes and bioactive compounds through high-throughput sequencing and LC-MS/MS analysis. The discovery of metabolites like acacetin and procyanidin, along with crucial enzymes in phenylpropanoid and flavonoid pathways, opens avenues for targeted metabolic engineering and screening of active compounds, enhancing its therapeutic applications.	https://www.mdpi.com/2073-4425/13/10/1909	2022

Sruthy Sathish	Chemical Papers	Identification of selective inhibitors for Janus kinase 1: an integrated drug repurposing strategy for breast cancer	Breast cancer is the most common type of cancer and is responsible for most cancer-related deaths. Existing breast cancer treatments have inherent drawbacks, reinforcing the need to develop new ones. JAK1 is required to activate the inflammatory cytokine IL-6 class by ERBB2 receptor tyrosine kinase signalling in breast cancer cells. Conjointly, JAK1 plays a significant role in the evolution of metastatic cancer and the incessant activation of STAT3 oncogene. This emphasizes that JAK1 can be used to target breast cancer. In this study, we performed virtual screening against the FDA subset of Zinc15 database to identify potent and selective drug compounds against JAK1 protein using computational approaches. Molecular docking by Autodock tools 1.5.7 was used to segregate the compounds based on binding affinity. Followed by cross-docking to substantiate the selectivity and DFT analysis to determine the inhibitory efficiency of compounds using B3LYP technique with the 6-31G (d,p) basis set in Gaussian 16. To validate molecular interactions between selected inhibitor compounds and JAK1 structure molecular dynamic simulations employing Gromacs 2016.3 have been done using Gromos96 2005 force field. In addition, binding free energy calculations for the JAK1-drug complexes were carried out using MM/PBSA approach. Prior to this, toxicity profile of the drugs were analysed. Results from this study have predicted exatecan, fosnetupitant and ubrogepant as viable drugs. Therefore, JAK1 inhibition has been suggested as a possible way to target breast cancer. Additional validation employing in vitro studies may aid in identifying the bioactivity of selected compounds, enabling their application in mitigating this disease condition.	2.2	https://link.springer.com/article/10.1007/s11696-023-03070-1	Chemical Papers
Sruthy Sathish	Phytomedicine plus	Potency of anti-fibrotic herbs on fibrogenesis: A theoretical evaluation	within organs and tissues. Anti-fibrotic treatment represents an unconquered area for drug development, with enormous potential. Herbal concoctions provide an interesting pool of potential modulators of this disease process.Bilar binding affinity to TGF-β receptor type 2 molecule and SMAD molecule when compared to Pirfenidone, signifying their therapeutic potential.Results Our study confirmed that plumbagin and ferulic acid can be used to target TGF; rhein and curcumin can be used to target SMAD and they have anti-fibrotic potential. Conclusions The phytocompounds identified could be used as an anti-fibrotic drug in the treatment of fibrotic disorders. Furthermore, invitro and invivo experiments are to be carried out to validate the anti-fibrotic activity of these molecules.		https://www.sciencedirect.com/science/article/pii/S2667031323000921	2023
Deepak Kumar, C.Hepsibah Priyadarshini, V. Sudha, Jositta Sherine, S. Harinipriya, Samanwita Pal	J. Pharmaceutical Sciences	Investigation of adsorption behavior of anticancer drug on zinc oxide nanoparticles: A Solid state NMR and Cyclic Voltammetry (CV) analysis		Drug delivery system	https://doi.org/10.1016/j.xphs.2021.08.003	2021
C. Hepsibah Priyadarshini, V. Sudha* and S. Harinipriya	Phys. Chem. Chem. Phys	Computational mechanistic insights on Ag2O as a host for Li in lithium-ion batteries		Battery Material & Mechanism	10.1039/d2cp01674e	2022
C. Hepsibah Priyadarshini, V. Sudha* and S. Harinipriya	J. Electrochem. Soc.	A DFT Approach and Perspective of Sodiation in Ag2O host – Exploration towards Sodium Batteries		Battery Material & Mechanism	10.1149/1945-7111/ acf0ec	2023

Kaushik A Palicha, Pavithra Loganathan, V. Sudha and S. Harinipriya	Sci. Reports	Non-Enzymatic biodegradable battery from plant-based microtubules cathode – Monte Carlo simulation and Experimental validation		Biobattery	https://doi.org/10.1038/s41598-023-36902-x	2023
Karunakaran M	Journal of Magnetism and Magnetic Materials	Ab-initio study of tuning the electronic and magnetic properties ofNi2MnGa Heusler alloy by Co and Mn compound doping	We report the effects of Mn and Co doping on the electronic properties, magnetic exchange interaction, andCurie temperature of intermetallic Ni2MnGa by Green’s function based Korringa–Kohn–Rostoker method withcoherent potential approximation(KKR-CPA). The effect of single and compound doping of Mn and Co atdifferent crystallographic positions on these properties are evaluated by computing the electronic and magneticstructures of Ni2MnGa. The study revealed the possibility of tuning magnetic exchange interaction andstructures of Ni2MnGa. The study revealed the possibility of tuning magnetic exchange interaction andstructures of Ni2MnGa. The study revealed the possibility of tuning magnetic exchange interaction and Curie temperature( ) upon doping. Moreover, it is noted that doping can stabilize the Jahn–Teller distortion.It is also worth noting that responds in a different way with concentration as well as the site of thedopant. This study helps in understanding and realizing the cause for magnetic properties in Ni2MnGa, andexperimental peers can also use it for further research on doped Ni2MnGa.	2.7	https://www.sciencedirect.com/science/article/abs/pii/S0304885323000689?via%3Dihub	2023
Karunakaran M	Journal of Physics and Chemistry of Solids	Controlling the electronic and magnetic properties of Mn2CoAl by metaldoping: A DFT studydoping: A DFT study	We report a computational investigation of the structural, electronic, and magnetic properties of disorderedMn2CoAl. We doped the Mn site of Mn2CoAl with various concentrations of Mn’s nearest neighbours in theperiodic table – namely Cr, Fe, Tc, and Re – to tune the magnetic behaviour of Mn2CoAl. We calculated theproperties of the system using density functional theory and mean-field theory. We tuned the Curie temperatureand magnetic moment as a function of the doping element concentration. We show that doping with morethan 2% 3 transition metals and more than 10% 4 and 5 transition metals leads to the collapse of spin-gapless semiconductor behaviour. We have established that the doping element’s radius and number of valenceelectrons are mainly responsible for this spin-gapless semiconductor behaviour.	4	https://www.sciencedirect.com/science/article/abs/pii/S0022369724000490?via%3Dihub	2024
Karunakaran M	Journal of Solid State Chemistry	material: Fe30Cr45V25 all d-metal Heusler alloy	Comprehensive study on the critical behavior and magnetocaloric properties of Fe30Cr45V25 is carried out. Theferromagnetic alloy undergoes a second-order magnetic phase transition at TC = 300 K. The critical exponents ofFe30Cr45V25 are β = 0.380, γ = 1.293, and δ = 4.389. Although the obtained exponents do not fall into anyconventional universal classes (slightly relatable with 3D Heisenberg type), they get renormalized around TC andobey the Widom scaling relation, ascribed to the reliability of the calculation. 3D Heisenberg type (isotropic) spinrange order. Further, the magnetic entropy change (ΔSm) and relative cooling power for an applied field ofalignment is suggested by the renormalization group approach. However, the interaction strength is of long-temperature range with negligible hysteresis, a favorable feature for solid-state regenerators.	3.3	https://www.sciencedirect.com/science/article/abs/pii/S0022459624000562?via%3Dihub	2024

Greeshma R	Pramana	Tuning electronic and magnetic properties of FeRh alloy by chemical and physical method	The electronic, magnetic and thermodynamic properties of ordered and chemically disordered FeRh alloy are studied using ab-initio methods. The equiatomic FeRh composition is reported for both ordered and disordered phases. Chemically disordered FeRh is reported and the effect of disorder on electronic and magnetic properties is discussed. Further, we have reported the effects of stress and strain in both the ordered and disordered phases. The result is only for the cubic phase, and no distortion has been taken into consideration. This study is motivated by the recent resurgence in the FeRh and is inspired by the fact that it is possible to sustain the barocaloric properties over the cycle. Hence, we have discussed the properties of FeRh with chemical disorder and pressure simultaneously to gain an insight into the compound effect and the interplay between them.	2.8	https://doi.org/10.1007/s12043-023-02567-4	2023
Shrestha Dutta	AIP Conferrence proceedings	A Study of Electronic and Magnetic Properties of Transition Metal Trihalides	We present the electronic and magnetic structure calculations of VCl3, VBr3, CrCl3 and CrBr3. The results are obtained by density functional theory with plane wave basis sets. The transition metal trihalides generally optimize either in trigonal or monoclinic structures. We have focused on the effect of symmetry on the electronic and magnetic properties of the systems. We have found that magnetic moments change considerably depending on the symmetry. Both CrX3 has shown a bandgap ≈ 2eV while the V based systems have shown half-metallic properties.	5.2	10.1016/j.colsu	2023
Dr. J. Arockia Selvi	Colloids and Surfaces A: Physicochemical and Engineering Aspects	Molecular interaction and corrosion inhibition of benzophenone and itsMolecular interaction and corrosion inhibition of benzophenone and its derivative on mild steel in 1 N HCl: Electrochemical, DFT and MD simulation studies Molecular interaction and corrosion inhibition of benzophenone and its derivative on mild steel in 1 N HCl: Electrochemical, DFT and MD simulation studies Molecular interaction and corrosion inhibition of benzophenone and its derivative on mild steel in 1 N HCl: Electrochemical, DFT and MD simulation studies	In this study, Benzophenone (BP) and 2-Aminobenzophenone (2-A.BP) were evaluated for the corrosion inhi�bition effect on mild steel in 1 N HCl solution with various temperatures ranging from 303 to 333 K using gravimetric analysis. Spectroscopic analysis, Potentiodynamic Polarization (PDP), Electrochemical Impedance Spectroscopy (EIS), and Atomic Force Microscopy (AFM) were used to investigate corrosion inhibition mechanism and surface morphology of the inhibited metal surface. The inhibition efficiency (IE) of the compound increased with an increase in the concentration of inhibitors from 160 to 280 ppm. The maximum inhibition efficiency of 2-A.BP and BP are 90 % and 78.75 % at an optimal concentration of 280 ppm at 303 K. Poten�tiodynamic polarization measurement indicates the inhibitor to be a mixed-type and predominantly anodic typeinhibitors. The inhibitors were adsorbed onto the mild steel surface via physisorption. The adsorption of inhibitor appears to function through Langmuir adsorption isotherm more appropriately. Scanning Electron Microscopy (SEM) with Energy Dispersive X-ray (EDAX) analysis confirmed the adsorption of inhibitor molecules, thus protecting the steel surface from being directly exposed to acidic ions. The results of the UV–visible spectroscopy furnished evidence of iron/inhibitor interactions. The mechanism of corrosion inhibition was further disclosed intheoretical investigation using density functional theory (DFT) and molecular dynamics (MD) simulation. DFTanalyses revealed that both BP and 2-A.BP interacted effectively by electron-sharing mechanism resulting an interfacial adsorption of BP and 2-A.BP on the Fe (110) surface. MD studies showed the binding energy of 2-A.BPis less than that of BP. This confirms that 2-A.BP acts more efficiently in its role as an inhibitor. As a consequence, the computational analysis provided substantial evidence for the experimental results.	4.6	016/j.matchen	2023

Dr. J. Arockia Selvi	Materials Chemistry and Physics	3-Phenylquinazolin-4(3H)-one via a renewable approach as an efficient corrosion inhibitor for mild steel in acid media	3-phenylquinazolin-4(3H)-one (3pq) an organic aza-heterocyclic compound synthesised using a renewablebiomass source, and the structure is subsequently confirmed using 1H NMR, 13C NMR and FT-IR spectroscopictechniques. The inhibition activity of 3pq was examined with a set of experiments like Weight loss measurements which provided a high inhibition efficiency (IE) of 90.0% and a low corrosion rate (CR) of 1.54 mm/y at 300 ppm. Electrochemical studies such as potentiodynamic polarization study confirmed the mixed inhibition activity of the inhibitor molecule with low corrosion current (icorr) value of 17.4 µA/cm2 in the presence of higher concentration of 3pq, and electrochemical impedance spectroscopy showed higher charge transfer resistance (Rct) value of 524.81 Ω cm2 and all these experiments have been used to examine 3pq's inhibiting capability for MS in 1 N HCl solution. The examined compound's ability to prevent corrosion is less effective in higher temperature. 3pq followed the Langmuir adsorption isotherm, which showed higher linearity than the Freundlich and Temkin adsorption isotherm models. The surface morphology was examined using scanning electron microscopy (SEM), which showed a smoother surface corresponding to the formation of a protective film signifying effective adsorption of inhibitor on MS surface, atomic force microscopy (AFM) signifies lower surface roughness (19.62 nm) in inhibited MS when compared to the uninhibited MS (81.63 nm) and Contact angle measurement explains the formation of the hydrophobic layer of 3pq on the surface of the MS in which the contact angle rises from 48.5◦ (uninhibited MS) to 99.7◦ (inhibited MS). UV–Visible spectroscopy (UV–Vis.) wasemployed to explain the complex formation of the inhibitor at the MS surface. X-ray photoelectron spectroscopy (XPS) and Fourier transform infra-red Spectroscopy (FTIR) was employed to confirm the effective adsorption of inhibitors on the MS surface. Additionally, computational studies based on Density functional theory (DFT) was employed to study the ability of 3pq to get adsorbed on the MS surface and found that 3pq has a perfect affinity	7.7	g/10.1016/j.jec	2024

Dr. J. Arockia Selvi	Journal of Environmental Chemical Engineering	Bifunctional properties of Acacia concinna pod as a natural surfactant-based eco-friendly benign corrosion inhibitor towards carbon steel protection in saline medium: Experimental and theoretical research	A facile approach has been targeted in combating both the electrochemical and microbial induced corrosion (MIC) using an eco-friendly surfactant-based plant extract, Acacia concinna pod extract (AcPE) as a corrosion inhibitor for carbon steel (CS) in saline medium (3.5% NaCl). The ethanolic extract from the pod of Acacia concinna was found to contain glycidyl oleate, a fatty acid-based phytochemical, analysed by Gas Chromatography-Mass Spectrometry (GC-MS) showed the dual inhibitory effect. The anti-corrosive effect of AcPE on CS with varying concentrations ranging from 50–400 ppm was investigated by Gravimetric, Potentiodynamic Polarisation (PDP), and Electrochemical Impedance Spectroscopy (EIS). The findings indicated that percentage inhibition efficiency (IE%) increased with an increase in concentration and showed an optimum IE of 93.8% at 200 ppm. However, with a further increase in concentration of AcPE, the IE % decreased. As a result, the efficiency of the corrosion inhibitor is said to be at its highest level when the inhibitor concentration approaches critical micelle concentration (CMC). Plots of Polarisation Resistance (Rp), Charge transfer resistance (Rct) vs inhibitor concentrations yielded a straight line with a slope, which drastically changed at the CMC of the inhibitor studied. PDP analysis revealed that AcPE acts as a mixed-type inhibitor. The adsorption of AcPE on CS followed Langmuir adsorption isotherm. The protective layer was analysed by Scanning Electron Microscopy with Energy Dispersive X-ray Spectroscopy (SEM-EDX), Atomic Force Microscopy (AFM), and Fourier-Transform Infrared spectroscopy (FT-IR). Density Functional Theory (DFT) calculations were utilized to predict the behaviour of inhibitor and to rationalize the experimental results. AcPE was evaluated as a potential biocide to mitigate the effects of MIC using the Colony Forming Units (CFU) assay, and the results showed a percentage	2.4	.1080/016942	2021
Dr. J. Arockia Selvi	Journal of Adhesion Science and Technology	Effect of alkyl chain length on the corrosionEffect of alkyl chain length on the corrosion inhibition of mild steel in a simulated hydrochloric acid medium by a phosphonium based inhibitorinhibition of mild steel in a simulated hydrochloricacid medium by a phosphonium based inhibitor	The corrosion inhibiting effect of three synthesised phosphonium containing ionic liquids of varying alkyl chain length, namely, butyltriphenyl phosphonium bromide (BTPPB), hexyltriphenyl phosphonium bromide (HTPPB) and hexadecyltriphenyl phosphonium bromide (HDTPPB) on mild steel, was evaluated in 1 M HCl medium. The corrosion inhibition performance was studied by gravimetric method, potentiodynamic polarization studies, electrochemical impedance spectroscopy and quantum chemical studies (DFT). However, the results of the SEM, AFM and contact angle tests confirmed that the protective layer formed on the mild steel. Furthermore, assessed the theoretical calculations for exploring the inhibition mechanism. A maximum of 95.77% inhibition efficiency was achieved using 250 ppm of HDTPPB. The obtained results showed that HDTPPB has greater inhibition ability than BTPPB and HTPPB. Adsorption studies obeyed the Langmuir adsorption isotherm. Moreover, the increased alkyl chain length of ionic liquids did increase their inhibition efficiency.	2.4	.1080/016942	2021

Dr. J. Arockia Selvi	Rasayan Journal of Chemistry	EVALUATION OF TETRA-n-BUTYLAMMONIUM BROMIDE AS CORROSION INHIBITOR FOR MILD STEEL IN 1N HCl MEDIUM: EXPERIMENTAL AND THEORETICAL INVESTIGATIONS	The corrosion inhibition behavior of Tetra-n-butylammonium bromide (TBAB) on mild steel (MS) in 1N HCl was investigated through experimental and theoretical studies. Inhibition efficiency is found to have increased by a rise in the concentration of TBAB. Experimental (weight loss study, potentiodynamic polarization, electrochemical impedance spectroscopy) results suggested that TBAB exhibits better inhibition efficiency. Thermodynamic studies were discussed. TBAB on the mild steel surface obey Langmuir adsorption isotherm. SEM and AFM studies confirm the adsorption and protective ability of TBAB on mild steel in 1N HCl medium. Formation of a protective layer on mild steel was characterized by FT-IR, UV-Visible and XRD studies. Furthermore, quantum chemical parameters were calculated. The results demonstrate the adsorption capability of TBAB on mild steel in 1N HCl medium. Quantum chemical calculations are in good agreement with results obtained from experimental methods.	1.12	g/10.31788/RJ	2020
Monirul Shaikh, Madhusudan Karmakar, Saurabh Ghosh	Physical Review B	Strain-tuned properties of hybrid improper ferroelectric superlattices through first-principles calculations and machine learning	The hybrid improper ferroelectricity is due to the trilinear coupling between three symmetric phonon modes, and the free energy of the system can be described as F tri ~ α Q 1 Q 2 Q P, where α is the coupling constant and Q 1 and Q 2 are the primary order parameters coupled to the polar mode Q P. In the case of P n m a symmetry, the Q 1 and Q 2 modes are rotation, Q Rot (a 0 a 0 c+), and tilt, Q Tilt (a− a− c 0), of BO 6 octahedra, respectively. Here, we perform density functional theory (DFT) calculations along with machine learning (ML) to investigate the effects of biaxial strain on the ferroelectric and magnetic properties for hybrid improper ferroelectric (LaFeO 3) 1/(LnFeO 3) 1 superlattices (SLs), where Ln represents Ce, Nd, Sm, Gd, Dy, Y, Tm, and Lu. We have investigated how the polarization, magnetization, and coupling coefficients are modified subject to the external strain.	4.036	Strain-tuned properties	2020
Monirul Shaikh, Aafreen Fathima, MJ Swamynadhan, Hena Das, Saurabh Ghosh	Chemistry of Materials	Investigation into cation-ordered magnetic polar double perovskite oxides	The technique of coupling cation ordering with other microscopic degrees of freedom was employed to induce magnetic polar phenomena within the materials belonging to the double perovskite oxide family represented by the chemical formula AA′BB′O6, i.e., by considering double cation occupancy at both the 12- and 6-fold oxygen coordinated A- and B- cation sites. Starting from a paraelectric material, La2MnNiO6, that exhibits ferromagnetic behavior near room temperature, we constructed a wide chemical composition space to search for prospective polar magnetic systems. Since we have employed the hybrid improper mechanism of ferroelectricity to induce polar phenomena in these perovskite oxides, ensuring the stability of the cation ordering within certain octahedral rotational pattern was our primary imperative	10.508	Investigation into Cation-Ordered	2021
Duo Wang, Monirul Shaikh, Saurabh Ghosh, Biplab Sanyal	Physical Review Materials	Duo Wang, Monirul Shaikh, Saurabh Ghosh, Biplab Sanyal	A-and B-site ordered quadruple perovskites with the chemical formula AA 3′ B 2 B 2′ O 12 can form with 1: 3 ratio at the A site. A unique feature of this specially ordered perovskite is that three different atomic sites (A′, B, and B′ sites) can all accommodate magnetic transition metals. As a consequence, multiple magnetic and electronic interactions can occur at A′, B, and/or B′ sites, giving rise to a series of intriguing physical phenomena. CaCu 3 Fe 2 Re 2 O 12 is a good example, which shows half-metallic electronic structure, large magnetization, and a very high Curie temperature. Here we investigated a series of ferrimagnetic (FiM) compounds ACu 3 Fe 2 Re 2 O 12 (A= Ca, Sr, Ba, Pb, Sc, Y, La) by using density functional theory and Monte Carlo simulations.	3.989	Prediction of half-metallic	2021

MJ Swamynadhan, Saurabh Ghosh	Physical Review Materials	Designing multifunctional two-dimensional layered transition metal phosphorous chalcogenides	Layered two-dimensional (2D) transition metal phosphorous chalcogenides (TMPCs) are now in intense research focus due to their interesting ferroelectric and magnetic properties and compatibility with 2D electronic devices. Here, we have employed first-principles density functional theory calculations to investigate the electric and magnetic properties of ABP 2 S 6 (A= Cu, Ni; B= Cr, Mn) TMPCs. We have systematically investigated four TMPCs compounds, namely, CuCrP 2 S 6, CuMnP 2 S 6, NiCrP 2 S 6, and NiMnP 2 S 6, and reported unusual antiferroelectric/ferroelectric (AFE/FE) and electronic properties. We have found a more stable ferroelectric state in van der Waals (vdW) gap with higher polarization compared to the usual ferroelectric phase in the insulating state.	3.989	Designing multifunctional two-dimensional	2021
Monirul Shaikh, Soumyajit Ghosh, Saurabh Ghosh	Materials Letters	Strain engineered structural and electronic properties of an organic-crystal through first-principles calculations	We use first-principles density functional theory (DFT) calculations to investigate the effects of strain on the properties of elastic organic 2, 6-dichlorobenzylidene-4-fluoro-3-nitroaniline (DFNA) crystal. Our results from DFT calculations are in agreement with the recent experimental results of elastic DFNA crystal. The systematic calculations on the criss-cross arrangement of the crystal show that π π stacking along with weak and dispersive non-covalent interactions play a pivotal role in stabilizing the structure. We consider the following interactions, namely type-I Cl Cl interaction, type-II F Cl interaction, and C–H O interaction, and investigate how the interactions are tuned subject to strain. Also,	3.423	Strain engineered structural	2021
Abhinandan Patra, Monirul Shaikh, Saurabh Ghosh, Dattatray J Late, Chandra Sekhar Rout	Sustainable Energy & Fuels	MoWS 2 nanosheets incorporated nanocarbons for high-energy-density pseudocapacitive negatrode material and hydrogen evolution reaction	The rapid population explosion and widespread use of non-renewable energy sources have led to preoccupations such as the energy crisis, which motivates us to find alternative energy supplies and further harness their output energy through energy storage devices. In this work, we have demonstrated hybrids incorporating MoWS2 and nanocarbon (MWCNT and rGO) as bifunctional materials, i.e., electrocatalyst and negatrode (negative electrode), for both energy conversion and storage applications. All the fabricated electrodes underwent various characterization techniques including pXRD, Raman spectroscopy, FESEM, HRTEM, XPS, and BET, and were later subjected to electrochemical and electrocatalytic measurements. The MoWS2 incorporating MWCNTs outperformed all the prepared materials, attaining a highest capacitance of 592 F g−1 at a current density of 0.2 A g−1.	6.367	MoWS2 nanosheets incorporated nanocarbons	2022
TR Naveen Kumar, M Swamynadhan, Saurabh Ghosh, B Neppolian	Sustainable Energy & Fuels	Boron-induced oxygen vacancies for methanol oxidation reaction: selectivity towards formate via non-noble metals	Bottlenecks in the commercialization of direct methanol fuel cells (DMFCs) involve the use of noble metal electrocatalysts, value-less by-product formation, and carbon dioxide (CO2) emission. Herein, we developed non-noble-based boron-doped nickel–cobalt oxide (B/NiCo2O4) catalysts with abundant oxygen vacancies for efficient methanol oxidation to value-added formate as the by-product. The B/NiCo2O4 catalyst demonstrated a maximum current density of 240 mA mg−1, which is 2.7 and 1.5 times higher than that of the pristine nickel–cobalt oxide (NiCo2O4) and Pt/C (platinum on carbon) composite, respectively, accompanied with 1000 cycles stability. More excitingly, the value-added formate was produced as a by-product with a faradaic efficiency of 54%. The high current density and selectivity towards formate are mainly due to the accessibility of numerous methanol molecules on the B/NiCo2O4	6.367	Boron-induced oxygen vacancies	2022

Mukaddar Sk, Saurabh Ghosh	RSC advances	Understanding the role of 5d electrons in ferromagnetism and spin-based transport properties of K 2 W (Cl/Br) 6 for spintronics and thermoelectric applications	In this article, we have systematically investigated the structural, electronic, magnetic, and spin-based thermoelectric properties of K2W(Cl/Br)6 by first-principles calculation. The obtained negative formation energy confirmed the thermodynamic stability of K2W(Cl/Br)6, while the tolerance factor calculation showed their cubic phase stability. In addition, we have estimated the elastic constants which confirmed the mechanical stability of K2W(Cl/Br)6. Further, the spin-polarized band structure and density of states calculations revealed the half-metallic nature with high Curie temperature (Tc) values of 613 K and 597 K for K2WCl6 and K2WBr6, respectively. Moreover, we have studied the temperature variation of thermoelectric properties such as kl, σ, ke, S, PF, and ZT. Such results showed that higher ZT values for spin-down channels are obtained from ultra-low ke, and high PF.	3.361	Understanding the role of 5d electrons	2022
Monirul Shaikh, Alessandro Stroppa, Saurabh Ghosh	Journal of Magnetism and Magnetic Materials	Defect induced ferromagnetism in a two-dimensional metal–organic framework	Two-dimensional ferromagnetic materials are potential candidates that can be integrated with the current nanoelectronic and spintronic device architecture. The latest trends in designing spintronic devices are mainly based on two-dimensional (2D) inorganic compounds. Here, we present a study based on first-principles density functional calculations where we design a 2D ferromagnetic material within the family of metal–organic frameworks. Starting from the inorganic CrI 3 compound, we demonstrate that a chromium-based metal– organic compound ie Cr (COOH) 3 can be stabilized in a ferromagnetic state compared to the other possible anti-ferromagnetic states. The proposed structure of Cr (COOH) 3 is found to be thermodynamically stable, but its dynamic stability could not be verified because of complexity into the structure.	2.993	Defect induced ferromagnetism	2022
Shrabani Panigrahi, Mukaddar Sk, Santanu Jana, Saurabh Ghosh, Jonas Deuermeier, Rodrigo Martins, Elvira Fortunato	ACS Applied Energy Materials	Tailoring the interface in high performance planar perovskite solar cell by ZnOS thin film	Charge-carrier recombination within the photoactive and charge extraction layers is one of the major obstacles to achieve high performance perovskite solar cells. Here, we demonstrate an ultrathin layer of ZnOS in between SnO2 and halide perovskite film that can effectively passivate the defects, suppressing the nonradiative recombination loss. It also helps to moderate the perovskite layer with increasing surface potential, which facilitates transferring the carriers from the perovskite to the hole transport layer, consequently providing an understanding of the bottom-up interfacial passivation of perovskite films. An enhancement of VOC 100 mV mainly causes the efficiency improvement from 17.22 to 19.4% in the combined SnO2–ZnOS based solar cell. In addition, we have performed a device modeling and theoretical analysis of these perovskite solar cells with and without the passivation layer.	6.959	Tailoring the interface in high performance	2022
Mukaddar Sk, Saurabh Ghosh	International Journal of Energy Research	First-principles investigation of structural, optoelectronic, and thermoelectric properties of Cs2Tl(As/Sb)I6	In this article, we have systematically investigated the structural, electronic, optical, and thermoelectric properties of Cs2Tl(As/Sb)I6. The obtained negative formation energy along without the presence of imaginary phonon frequency confirmed the thermodynamic stability of Cs2Tl(As/Sb)I6. In addition, the new mBJ approach showed the direct band gap value of 1.10 and 1.33 eV for Cs2TlAsI6 and Cs2TlSbI6, respectively. Furthermore, the dispersed direct band nature of Cs2Tl(As/Sb)I6 leads to their outshining optical properties such as higher-order (105 cm−1) absorption coefficient, appreciable optical conductivity, and low reflectivity. Moreover, the higher figure of merit values of Cs2Tl(As/Sb)I6 are resulted from their ultra-low thermal conductivity and high electrical conductivity. Thus, Cs2Tl(As/Sb)I6 are predicted to be potential photovoltaic and thermoelectric materials.	5.164	thermoelectric properties of Cs2Tl(As/Sb)I6	2022

Gourav, Mukaddar Sk, Krishnamoorthy Ramachandran, Saurabh Ghosh	International Journal of Quantum Chemistry	First-principles investigation of Rb2Ag(Ga/In)Br6 for thermoelectric and photovoltaic applications	In this article, we have systematically investigated the structural, electronic, optical and thermoelectric properties of Rb2Ag(Ga/In)Br6. The resulting negative formation energy along with the absence of imaginary phonon modes confirm the thermodynamic stability of Rb2Ag(Ga/In)Br6. In addition, the derived electronic properties by using GGA-PBE + mBJ + SOC functional show that the direct band gap values are 1.21 eV and 1.42 eV for Rb2AgGaBr6 and Rb2AgInBr6, respectively. Furthermore, the dispersed direct band nature of Rb2Ag(Ga/In)Br6 leads to their outshining optical properties such as higher order (105 cm−1) absorption coefficient, appreciable optical conductivity, and low reflectivity. Moreover, the higher figure of merit values of Rb2Ag(Ga/In)Br6 are resulted from their ultra-low thermal conductivity and high electrical conductivity.	2.444	Rb2Ag(Ga/In) Br6 for thermoelectric	2022
Darin Joseph, Monirul Shaikh, Sathiyamoorthy Buvaneswaran, Trilochan Sahoo, Ayana Ghosh, Saurabh Ghosh	The Journal of Physical Chemistry C	First-Principles Study of Ferroelectric and Optical Properties in Derivatives of Thiourea	Organic ferroelectric materials in the form of molecular crystals are promising alternatives to well-known ferroelectric perovskite oxides due to their structural flexibility, tunability, and ease of processing. First-principles density functional theory calculations combined with group theory analyses are employed in this work to discuss polar nature of a class of derivatives of thiourea: CH4N2A where A = O, S, Se, and Te. Optical properties in the UV range along with thermodynamic and dynamic stability of such materials are also evaluated in the study. We find that CH4N2Te with bandgap energy of 3.33 eV shows large spontaneous polarization of P = 10.92 µC/cm2. The electronic and optical properties become tunable under strain.	4.126	Properties in Derivatives of Thiourea	2022
Ayana Ghosh, Gayathri Palanichamy, Dennis P Trujillo, Monirul Shaikh, Saurabh Ghosh	Chemistry of Materials	Insights into cation ordering of double perovskite oxides from machine learning and causal relations	This work investigates origins of cation ordering in double perovskites using first-principles theory computations combined with machine learning (ML) and causal relations. We have considered various oxidation states of A, A′, B, and B′ from the family of transition metal ions to construct a diverse compositional space. A conventional framework employing traditional ML classification algorithms such as Random Forest (RF) coupled with appropriate features including geometry-driven and key structural modes leads to accurate prediction (98%) of A-site cation ordering. We have evaluated the accuracy of ML models by employing analyses of decision paths, assignments of probabilistic confidence bound, and finally a direct non-Gaussian acyclic structural equation model to investigate causality. Our study suggests that structural modes are crucial for classifying layered, columnar, and rock-salt ordering.	10.508	Insights into cation ordering	2022
Mukaddar Sk, Saurabh Ghosh	Optik	16.35% efficient Cs2GeSnCl6 based heterojunction solar cell with hole-blocking SnO2 layer: DFT and SCAPS-1D simulation	Cs2GeSnCl6 is predicted to be an emerging material for the construction of high-efficiency solar cells. In this article, we have explored the structural, optoelectronic and photovoltaic properties of Cs2GeSnCl6 by using first-principles and SCAPS-1D simulations. The formation energy and phonon band structure calculations confirmed the thermodynamic stability of Cs2GeSnCl6. The electronic property of Cs2GeSnCl6 revealed a direct band gap of 0.91 eV (with SOC) by using the mBJ exchange-correlation functional. The optical calculations ensured a high absorption coefficient and low reflectance. Furthermore, the simulated photovoltaic performance of Cs2GeSnCl6-based heterojunction solar cell i.e. ITO/SnO2/ Cs2GeSnCl6/Au shows the optimum PCE (%) of 16.35 %, which is higher than the recently predicted PEC (%) value from Cs2AgBiBr6 based solar cell.	3.1	Cs2GeSnCl6 based heterojunction	2022

Abinaya Stalinraja, Keerthiga Gopalram, Srinivasadesikan Venkatesan, MJ Swamynathan, Saurabh Ghosh, Tamilmani Selvaraj	Electrochimica Acta	Electrochemical reduction of CO2 on Cu doped titanium nanotubes—an insight on ethylene selectivity	Electrochemical reduction of CO2 is performed on Cu electrodeposited Ti nanotubes (Cu/TiNT). TiNT is prepared by anodization method followed by electrodeposition of Cu and the CO2 reduction achieved is compared with that of bare electrodes. The comparison between Cu/TiNT and TiNT is done based on the characterization techniques of Scanning Electron Microscopy, X-ray Diffraction, Transmission Electron Microscopy, X-ray Photoelectron Spectroscopy and UV-Diffuse Reflectance Spectroscopy. Electrochemical reduction of CO2 is carried out in an H-type cell with 0.5 M KCl electrolyte, and ethylene, methane, formic acid, CO, hydrogen along with methanol and ethanol are observed as trace products. Among the electrodes studied, maximum Faradaic efficiency (55%) is observed for Cu/TiNT compared to TiNT and bare electrodes.	6.901	Electrochemical reduction of CO2	2022
Rodrigo Ferreira, Monirul Shaikh, Suresh Kumar Jakka, Jonas Deuermeier, Pedro Barquinha, Saurabh Ghosh, Elvira Fortunato, Rodrigo Martins, Santanu Jana	Nano Letters	Bandlike Transport in FaPbBr3 Quantum Dot Phototransistor with High Hole Mobility and Ultrahigh Photodetectivity	Halide perovskites have been widely explored for numerous optoelectronic applications among which phototransistors have appeared as one of the most promising light signal detectors. However, it is still a great challenge to endow halide perovskites with both mobility and high photosensitivity because of their high sensitivity to moisture in ambient atmosphere. Here, we explore an FAPbBr3 perovskite quantum dot (QD) phototransistor with bandlike charge transport and measure a dark hole mobility of 14.2 cm2 V–1 s–1 at ambient atmosphere. Attaining both high mobility and good optical figures of merit, a detectivity of 1016 Jones is achieved, which is a record for halide perovskite nanocrystals. Simple A-site salt (FABr) treatments offer a mechanism for connecting between perovskite QDs for better charge transfer in high-quality devices.	10.8	Bandlike Transport in FaPbBr3	2022
MJ Swamynadhan, Ayana Ghosh, Saurabh Ghosh	Materials Horizons	Design of high polarization low switching barrier hybrid improper ferroelectric perovskite oxide superlattices	Hybrid improper ferroelectricity is a useful tool to design ABO3/A'BO3 polar superlattices from non polar building blocks. In this study, we have designed high polarization-low switching barrier hybrid improper ferroelectric superlattices with efficient polarization, and polarization-magnetization switching properties above room temperature, using density functional theory and ab initio molecular dynamics simulations. Superlattices with a chemical formula of (AAlO3)m/(A'AlO3)n, where m/n = 1/1, 1/3, 3/1, 1/5 and 5/1, A, A' = Lanthanide and Y cations are considered to outline the design principles behind polarization switching and (LaFeO3)3/(CeFeO3)1 is investigated for polarization-magnetization switching. We find that the unconventional switching paths via out-of-phase rotation QR− (a0a0c−) and tilt precession QTP always yield lower switching barrier compared to those via in-phase rotation QR+ (a0a0c+)	14.356	Design of high polarization low switching barrier	2023
Aafreen Fathima, Monirul Shaikh, Saurabh Ghosh	Physica B: Condensed Matter	Functional properties of A-site cation ordered phases derived from La2MnNiO6 double perovskites	Starting from a room temperature parent La 2 MnNiO 6 double perovskite as a prototype example, we ventured ferroelectricity and metal–insulator transition in the AA' BB' O 6 double perovskites. Using first-principles density functional calculations guided by symmetry, we have shown that by appropriate A-site substitution ie, by forming AA' combinations, La 2 MnNiO 6 within Mn and Ni in rock-salt ordering can be transformed into both ferroelectric insulating or polar metallic phase. We found that the charge difference between the cations and the radius mismatch between A and A' are the key factors for deciding a particular ordering. The layered ordering becomes more stable when both charge difference and radius mismatch are large. The energy gain is more pronounced when the charge difference at the A-site is large.	2.436	La2MnNiO6 double perovskites	2023

Sathiyamoorthy Buvaneswaran, Monirul Shaikh, Rajan Gowsalya, Trilochan Sahoo, Saurabh Ghosh	The Journal of Physical Chemistry C	Design of Ferroelectric Double Perovskite Oxides as Photovoltaic Materials	In ferroelectric-based photovoltaic materials, spontaneous polarization is expected to couple with the electronic and optical properties of the materials, and such materials have drawn attention as photovoltaic solar cells. Here, we utilize hybrid improper ferroelectricity to induce ferroelectric polarization in selected A-site layered and B-site rock-salt AA’BB’O6 double perovskites and propose an alternate route to design ferroelectric photovoltaic semiconductors. First-principles density functional theory calculations and ab initio molecular dynamics simulations are performed to investigate the optical, electronic, and ferroelectric properties. We consider RbLaMnWO6 and RbYMnWO6 as model systems to pursue this study. We identify that these materials are semiconductors with a minimalist forbidden energy gap (Eg) of 2.31 and 2.14 eV, respectively.	4.126	Photovoltaic Materials	2023
Haining Zheng, Arup Ghosh, MJ Swamynadhan, Gang Wang, Qihan Zhang, Xiao Wu, Ibrahim Abdelwahab, Walter PD Wong, Qing-Hua Xu, Saurabh Ghosh, Jingsheng Chen, Branton J Campbell, Alessandro Stroppa, Junhao Lin, Ramanathan Mahendiran, Kian Ping Loh	Journal of the American Chemical Society	Electron spin decoherence dynamics in magnetic manganese hybrid organic–inorganic crystals: the effect of lattice dimensionality	Organic–inorganic metal hybrids with their tailorable lattice dimensionality and intrinsic spin-splitting properties are interesting material platforms for spintronic applications. While the spin decoherence process is extensively studied in lead- and tin-based hybrids, these systems generally show short spin decoherence lifetimes, and their correlation with the lattice framework is still not well-understood. Herein, we synthesized magnetic manganese hybrid single crystals of (4-fluorobenzylamine)2MnCl4, ((R)-3-fluoropyrrolidinium)MnCl3, and (pyrrolidinium)2MnCl4, which represent a change in lattice dimensionality from 2D and 1D to 0D, and studied their spin decoherence processes using continuous-wave electron spin resonance spectroscopy.	15.419	Manganese Hybrid Organic–Inorganic Crystals	2023
Palanichamy Gayathri, MJ Swamynathan, Monirul Shaikh, Ayana Ghosh, Saurabh Ghosh	Chemistry of Materials	Switching of Hybrid Improper Ferroelectricity in Oxide Double Perovskites	In ABO3-type perovskite oxides with Pnma symmetry, rotation (QR+, a0a0c+) and tilt (QT, a–a–c0) of BO6 octahedra are the two primary order parameters. These order parameters establish an inherent trilinear coupling with anti-ferroelectric A-site displacement (QAFE) to form the low-symmetry phase. The symmetry is further lowered in double perovskite oxides (DPOs) due to A/A’ cation ordering. It in turn makes these systems polar via hybrid improper ferroelectric mechanism, primarily driven by QR+ and QT. Naturally, it has been believed that functionalities such as polarization can also be switched by tuning these primary order parameters. However, mystery around finding switching mechanism still remains. Our study based on density functional theory calculations combined with finite-temperature molecular dynamics simulations shows that the polarization switching is a two-step process, driven by out-of-phase …	10.508	Switching of Hybrid Improper Ferroelectricity	2023

Ayana Ghosh, Dennis P. Trujillo, Subhashis Hazarika, Elizabeth Schiesser, M. J. Swamynathan, Saurabh Ghosh, Jian-Xin Zhu, Serge Nakhmanson	APL Mach. Learn.	Identification of novel organic polar materials: A machine learning study with importance sampling	Recent advances in the synthesis of polar molecular materials have produced practical alternatives to ferroelectric ceramics, opening up exciting new avenues for their incorporation into modern electronic devices. However, in order to realize the full potential of polar polymer and molecular crystals for modern technological applications, it is paramount to assemble and evaluate all the available data for such compounds, identifying descriptors that could be associated with an emergence of ferroelectricity. In this paper, we utilized data-driven approaches to judiciously shortlist candidate materials from a wide chemical space that could possess ferroelectric functionalities. A machine learning study with importance sampling was employed to address the challenge of having a limited amount of available data on already-known organic ferroelectrics. Sets of molecular-and crystal-level descriptors were combined with a …	-	Identification of novel organic polar materials	2023
Rajan Gowsalya, Monirul Shaikh, Saurabh Ghosh	Journal of Magnetism and Magnetic Materials	Designing ferromagnetic polar half-metals in short-period perovskite nickelates	ABO 3 perovskites oxides show fascinating functional properties, including ferroelectricity, magnetism, metal-to-insulator transition, half metallicity, polar metallic phase, etc. In particular, rare earth nickelates and alkaline earth nickelates within the orthorhombic crystal structures show an insulator–metal transition (IMT) and half-metallic (HM) nature respectively. Here, we report a series of ferromagnetic polar half metals by constructing LnNiO 3/CaNiO 3 short period 1/1 superlattices (SLs) with Ln= La, Nd, Gd, Dy, Tm, and Lu within an orthorhombic phase. The polar distortion is induced by a hybrid-improper ferroelectric mechanism ie, by constructing Ln/Ca layer-ordering. The system shows a ferromagnetic Ni-Ni interaction, whereas Ni-3 d's are interacting antiferromagnetically with O-2 p. We explain that the origin of observed half metallicity and ferromagnetism is due to strong hybridization between Ni-3 d and O-2 p …	2.993	Designing ferromagnetic polar half-metals	2023
Palanichamy Gayathri, Saurabh Ghosh, Ayana Ghosh	Chemistry of Materials	Predictive Design of Hybrid Improper Ferroelectric Double Perovskite Oxides	The computational design of suitable multiferroic double perovskite oxides requires finding materials that exhibit sizable polarization, magnetization, and coupling between them. Oxides with the chemical formula of AA'BB'O6 with building blocks of ABO3 single perovskite oxides in centrosymmetric Pnma symmetry are strong candidates that have been reported to satisfy such criteria. The system lowers to noncentrosymmetric, polar P21 symmetry if A/A' layered and B/B' rocksalt cation orderings are imposed. A detailed compositional search over a variety of chemical spaces followed by evaluating their polarization may lead to the identification of more of these compounds with ferroelectric ordering. The standard density functional theory practices to estimate polarization within the Berry phase formalism require the systems to be perfectly insulating. The number of compounds that can be evaluated using this …	10.508	Predictive Design of Hybrid Improper Ferroelectric	2023
Sakthi Balaji A	Physical Chemistry Chemical Physics	Experimental and theoretical insights into supercapacitive performance of interconnected WS2 nanosheet	Transition metal dichalcogenides (TMDs) are fascinating and prodigious considerations in the electrochemical energy storage sector because of their two/dimensional chemistry as well as heterogeneous characteristics. Herein, we synthesized interconnected WS2 nanosheets by hydrothermal method followed by the sulphuration at 850 oC in an argon atmosphere. The ultrathin WS2 nanosheet array is endowed with an excellent specific capacitance of 74 F g-1 at the current density of 3 A g-1 up 7000 cycles. Moreover, a symmetric supercapacitor was fabricated using WS2 nanosheets which provided the admirable high specific capacity of 6.3 F g-1 at 0.05 A g¬1 with the energy and power density of 5.6 x 102 mWh kg-1 and 3.6 x 105 mWkg-1, respectively. Density Functional Theory (DFT) simulations revealed the presence of populated energy states near the Fermi level resulting in a high quantum capacitance value which supports the experimentally achieved high capacitance value. The attained results recommend interconnected WS2 nanosheets as a novel, robust, and low-cost electrode material for supercapacitor energy storage devices.	3.676	https://pubs.rsc.org/en/content/articlehtml/2024/cp/d4cp00206g	2024

Article (Tumpa)	New Journal of Chemistry	Metal–organic framework-catalyzed selective oxidation of alcohols and oxidative cross-coupling for C–C and C–N bond-forming reactions	A novel porous metal–organic framework Co(btc)(bpy) (Co-MOF-3a) was synthesized by employing a bipyridyl ligand, benzene tricarboxylic acid, and Co(NO3)2·6H2O and was completely characterized. The mesoporous nature of the MOF catalyst was confirmed using BET measurements. The confirmation of the proposed structure of Co-MOF-3a was also supported through a computational study. This MOF could serve as a highly efficient heterogeneous catalyst for the oxidation of a variety of alcohols with tert-butyl hydroperoxide (t-BuOOH) as an oxidant. Furthermore, the current catalytic approach facilitated the oxidative coupling reaction in one pot to obtain a wide range of biologically important molecules, such as benzimidazole, benzothiazole, quinozolones, and arylidene malononitrile. The high performance of the MOF could be due to the presence of both the metal and carboxylate group of the ligand. The recyclability and scalability of the catalyst was found to be efficient and suitable for commercial applications.	3.3	https://pubs.rsc.org/en/content/articlelanding/2024/nj/d3nj05260e/unauth	2024
Article(Tumpa)	The Journal of Physical Chemistry B	Density Functional Theory-Guided Photo-Triggered Anticancer Activity of Curcumin-Based Zinc (II) Complexes	Photodynamic therapy (PDT) has evolved as a new therapeutic modality for cancer treatment with fewer side effects and drug resistance. Curcumin exhibits PDT activity, but its low bioavailability restricts its clinical application. Here, the bioavailability of curcumin was increased by its complex formation with the Zn(II) center. For a structure–activity relationship study, Zn(II)-based complexes (1–3) comprising N^N-based ligands (2,2′-bipyridine in 1 and 2 or 1,10-phenanthroline in 3) and O^O-based ligands (acetylacetone in 1, monoanionic curcumin in 2 and 3) were synthesized and thoroughly characterized. The X-ray structure of the control complex, 1, indicated a square pyramidal shape of the molecules. Photophysical and TD-DFT studies indicated the potential of 2 and 3 as good visible light type-II photosensitizers for PDT. Guided by the TD-DFT studies, the low-energy visible light-triggered singlet oxygen (1O2) generation efficacy of 2 and 3 was explored in solution and in cancer cells. As predicted by the TD-DFT calculations, these complexes produced 1O2 efficiently in the cytosol of MCF-7 cancer cells and ultimately displayed excellent apoptotic anticancer activity in the presence of light. Moreover, the molecular docking investigation showed that complexes 2 and 3 have very good binding affinities with caspase-9 and p-53 proteins and could activate them for cellular apoptosis. Further molecular dynamics simulations confirmed the stability of 3 in the caspase-9 protein binding site.	3.466	https://pubs.acs.org/doi/abs/10.1021/acs.jpcb.3c02382	2023
Kathirvel Venugopal	Materials Letters	Thermoelectric properties of Lenaite: A first principles study	The electronic and transport properties of AgFeS2 were studied using first principles. The stable magnetic state of the material was found as antiferromagnetic. The band structure and DOS was calculated. The calculations show that the AgFeS2 system has an indirect bandgap of 0.94 eV. The transport properties were studied using the BoltzTraP2 code by solving the semiclassical Boltzmann transport equation. The orientation dependent transport properties of lenaite with respect to relaxation time shows moderate Seebeck coefficient, electrical conductivity, thermal conductivity, and power factor in y-direction. Our study reveals the high Seebeck coefficient of 1542 µV/ K and power factor of 1.93 × 1011 W/mK2s, respectively, for the p-type counterpart. These results show that pdoped AgFeS2 will be a potential candidate for thermoelectric applications.	3	https://www.sciencedirect.com/science/article/abs/pii/S0167577X21008430?via%3Dihub	2021

Kathirvel Venugopal	RSC advances	Pressure-driven thermoelectric properties of defect chalcopyrite structured ZnGa2Te4: ab initio study	The pressure induced structural, electronic, transport, and lattice dynamical properties of ZnGa2Te4 were investigated with the combination of density functional theory, Boltzmann transport theory and a modified Debye–Callaway model. The structural transition from I4 to �I42 �m occurs at 12.09 GPa. From the basic observations, ZnGa2Te4 is found to be mechanically as well as thermodynamically stable and ductile up to 12 GPa. The direct band gap of 1.01 eV is inferred from the electronic band structure. The quantitative analysis of electron transport properties shows that ZnGa2Te4 has moderate Seebeck coefficient and electrical conductivity under high pressure, which resulted in a large power factor of 0.63 mW m�1 K�2 (750 K). The ultralow lattice thermal conductivity (�1 W m�1 K�1 at 12 GPa) is attributed to the overlapping of acoustic and optical phonon branches. As a result, the optimal figure of merit of 0.77 (750 K) is achieved by applying a pressure of 12 GPa. These findings support that ZnGa2Te4 can be a potential p-type thermoelectric material under high pressure and thus open the door for its experimental exploration.	4.04	https://pubs.rsc.org/en/content/articlehtml/2022/ra/d2ra00805j	2022
Kathirvel Venugopal	Computational Materials Science	Thermoelectric power factor of MnSb2X4 (X= S, Se) spinel chalcogenides–A DFT study	Recently, spinel chalcogenides have been found to be promising class of materials in thermoelectric power generation. In this line, the complete understanding about electronic and thermoelectric properties of MnSb2S4 and MnSb2Se4 is crucial. With the help of first-principles calculations, its interesting characteristics are explored, including bonding nature, ground state magnetic ordering, mechanical stability, etc. A systematic study on these materials revealed their antiferromagnetic and semiconducting behaviour. The Seebeck coefficient as a function of carrier concentration has its maximum at 600 and 681 µV K−1 (T = 300 K) for hole doped MnSb2S4 and MnSb2Se4 respectively. Besides the coupled behaviour of Seebeck coefficient and electrical conductivity, an optimal power factor of 1.82 and 0.96 mW m−1 K−2 is attained at 300 K for MnSb2S4 and MnSb2Se4 respectively. This study suggests that both the spinels can be potential p-type thermoelectric materials for near room temperature power generation applications and enables the path for their experimental investigations.	3.3	https://www.sciencedirect.com/science/article/abs/pii/S0927025622004712	2022
Kathirvel Venugopal	Journal of Alloys and Compounds	Intrinsic ultra-low lattice thermal conductivity in orthorhombic BiSI: An excellent thermoelectric material	Eco-friendly chalcohalide compounds composed by heavy elements are the interesting candidates for thermoelectric energy conversion applications due to their intrinsically low lattice thermal conductivity, abundance and semiconducting behavior. This piqued the present study to investigate BiSI chacohalide for its feasibility in thermoelectric conversion through first principles computations. The deep insights into mechanical and lattice dynamical properties exposes the stability of BiSI. The transport properties of BiSI as a ~ function of carrier concentration builds noticeable power factor of 1.3 mW m−1 K−2 (300 K) and and 1.9 mW m−1 K−2 (500 K). The calculated lattice thermal conductivity of BiSI is 0.2 W m−1 K−1 at 300 K. This low kL can be resulted from phonon-phonon scattering process promoted by strong coupling between acoustic-optical branches. Moreover, the optimal figure of merit of 1.1–2.5 is observed at 300–500 K for both p- and n-type BiSI. The current study provides evidence for orthorhombic BiSI as a potentially beneficial thermoelectric material for room-to-mid temperature applications and it also accomplishes a gravitation towards pertinent experimental investigations.	6.2	https://www.sciencedirect.com/science/article/abs/pii/S0925838822037380	2022

Kathirvel Venugopal	Materials Chemistry and Physics	Role of lattice thermal conductivity in thermoelectric properties of chalcopyrite-type antimonides XSiSb2 (X= Mg, Be): A DFT insight	The widely available low-cost materials with high performance acts as a great choice for thermoelectric energy conversion applications. Here, the thermoelectric properties of two environmentally friendly chalcopyrites namely, MgSiSb2 and BeSiSb2 with tetragonal crystal structure, is investigated systematically. With the help of first principles combined with Boltzmann transport equations and modified Debye-Callaway model, electronic and thermal transport properties are studied. From electronic structures, it is inferred that both the chalcopyrites falls under semiconducting region with narrow band gap. The phonon dispersions suggest that these antimonides are thermodynamically stable with strongly coupled acoustic and optical mode of vibrations. Moreover, MgSiSb2 has high figure of merit (zT) of 2.06 (n = 1 × 1020 cm−3) with ultralow lattice thermal conductivity (kL) of 1.01 W m−1 K−1 at 900 K, whereas, BeSiSb2 has low zT of 0.23 due to its larger kL. Besides, these results demonstrate that this prediction can pave the way for experimental explorations.	4.6	https://www.sciencedirect.com/science/article/abs/pii/S0254058422014961	2023
Kathirvel Venugopal	Materials Science in Semiconductor Processing	Efficacy of pyrostilpnite (Ag3SbS3) mineral as thermoelectric material: A first principles study	Recently, environmental-friendly chalcogenides composed of cost-effective elements began contributing its proportion to the thermoelectric (TE) industry attributed to its greater conversion efficiency. On the track of exploration, suitability of pyrostilpnite (Ag3SbS3), a naturally available semiconducting mineral is investigated for TE applications using density functional and Boltzmann transport theory. The electronic band structure unveils its indirect band gap of 1.54 eV with favourable band feature (i.e.): degenerate flat bands resulting constructive carrier effective masses. Likewise, the reasonable Seebeck coefficient as well as electrical conductivity yields noticeable power factor of 1.611 mW m−1 K−2 at optimum electron concentration. Besides, the calculated lattice thermal conductivity reaches 0.392 W m−1 K−1 at 900 K. The synergetic effect of PF and kL intensely elevated the figure of merit to 1.64 at 900 K. The current study manifests eco-friendly pyrostilpnite mineral as a potentially beneficial candidate for TE devices and it could act as the waymark for experimental investigations.	4.1	https://www.sciencedirect.com/science/article/abs/pii/S1369800123002068	2023
Kathirvel Venugopal	Journal of Solid State Chemistry	Ordered-vacancy defect chalcopyrite ZnIn2Te4: A potential thermoelectric material with low lattice thermal conductivity	An effective route towards commercializing thermoelectric devices is to explore materials with high conversion efficiency. This study investigates the thermoelectric properties of ZnIn2Te4 with the combination of first-principles calculations, Boltzmann transport theory and the modified Debye Callaway model. This vacancy-ordered defect chalcopyrite shows a direct band gap of 1.37 eV, obtained by mBJ functional with spin orbit coupling. The positive phonon dispersion curves ensure the thermodynamical stability of the material. Moreover, strong acoustic-optical coupling, Grüneisen parameter, and moderate phonon group velocity yielded the low lattice thermal conductivity (kL) of 1.46 W m−1 K−1 at 900 K. Owing to this low kL, the optimum thermoelectric figure of merit of 0.90 and 0.98 is obtained for p and n-type ZnIn2Te4. These findings will open the way for the experimentalists to attempt for its experimental realization.	3.3	https://www.sciencedirect.com/science/article/abs/pii/S002245962300244X	2023

Kathirvel Venugopal	ACS Applied Energy Materials	Anisotropic Electron and Phonon Transport Properties in Pnictogen Chalcohalides: PnSI (Pn= Sb, Bi)	Semiconducting heavy pnictogen-containing chalcohalides are gaining wide attention in thermoelectrics, ascribed to their inherently low thermal conductivity. The present work uses first-principles computations to report the excellent thermoelectric performance of weak van der Waals 1D PnSI (Pn = Sb, Bi) crystals. Considering the substantial anisotropy in the crystal structure, the direction-dependent electron and phonon transport properties are studied. At 500 K, SbSI and BiSI exhibit ultralow lattice thermal conductivities (kL) of 0.260 W m–1 K–1 (0.428 W m–1 K–1) and 0.182 W m–1 K–1 (0.311 W m–1 K–1) along the x-direction (y-direction). Simultaneously, the moderate power factors of 4.03 (12.19) and 4.43 (7.91) mW m–1 K–2 are realized at specific hole concentrations under similar conditions. Eventually, the combination of ultralow kL and moderate power factor in the y-direction turned into excellent figure of merit, zT of 1.97 (1.78) and 2.71 (1.71) at 500 K with 7.0 × 1019 (2.7 × 1019) and 4.4 × 1019 (2.0 × 1019) cm–3 carriers for p-type (n-type) SbSI and BiSI, respectively. Therefore, both chalcohalides can rival the existing mid-temperature thermoelectric materials.	6.4	https://pubs.acs.org/doi/abs/10.1021/acsaem.3c01811	2023
Kathirvel Venugopal	Physical Chemistry Chemical Physics	One-dimensional van der Waals BiSBr: an anisotropic thermoelectric mineral	The fascinating characteristics of one-dimensional van der Waals crystals (V–VI–VII) enable their wide functionality. In particular, their anisotropic carrier transport and low thermal conductivity are advantageous from a thermoelectric viewpoint. In a quest for the "electron crystal phonon glass" paradigm, the present work investigated the thermoelectric performance of BiSBr. Deep insights were gained into the structural and electronic properties that revealed the synergetic effect of the bonding heterogeneity, lone pair of electrons, and degenerated bands that accelerated favorable transportation. Consequently, a low lattice thermal conductivity (0.225 W m−1 K−1) and considerable power factor (3.471 mW m−1 K−2) and thus a high zT of 2.34 were noted in the x-direction (perpendicular to the chain) at 500 K in the case of the material with 1.5 × 1020 holes per cm3. These observations suggest that BiSBr is a plausible near-room-temperature anisotropic thermoelectric mineral.	3.3	https://pubs.rsc.org/en/content/articlelanding/2024/cp/d3cp05849b/unauth	2024
Kathirvel Venugopal	Computational Materials Science	Lenaite (AgFeS2): A dynamically stable mineral with excellent thermoelectric performance	Diamond-like chalcopyrites have gained superior attention in thermoelectrics due to their attractive thermal transportation. On the mark of exploring environmental-friendly thermoelectric (TE) materials, this work unveils the suitability of lenaite (AgFeS2) through first-principles calculations. Owing to the beneficial band features leading to favourable effective mass, AgFeS2 exhibits good electron transport characteristics. Concurrently, the ultra-low lattice thermal conductivity of 0.47 W m−1 K−1 is realized at 500 K; ascribed to the large Grüneisen parameter, moderate phonon velocity, and Debye temperature. The combinations of these transport properties yield significant figure of merit of 0.87 at 500 K for 1.39 × 1020 holes per cm3. This study not only emphasis the TE properties of lenaite but also facilitates to understand its fundamental properties, including structural, electron and phonon-related properties.	3.3	https://www.sciencedirect.com/science/article/abs/pii/S0927025623007000	2024

Kathirvel Venugopal	ACS Applied Energy Materials	Sulfur Vacancy-Driven Band Splitting and Phonon Anharmonicity Enhance the Thermoelectric Performance in n-Type CuFeS2	Ternary chalcogenides of CuFeS2–x (x = 0.00–0.20) chalcopyrites were synthesized via vacuum melting reaction/uniaxial hot pressing, and their thermoelectrical properties were investigated at temperatures ranging from 315 to 605 K. The crystal structures and microstructures of all samples were examined using powder X-ray diffraction and scanning electron microscopy, respectively. X-ray photoelectron spectroscopy (XPS) was utilized to validate the oxidation states of Cu1+, Fe3+, and S2– in CuFeS2–x. As sulfur vacancy increased, the power factor, S2σ, increased from 0.18 mW/mK2 for CuFeS2 to 0.20 mW/mK2 for CuFeS1.8 at 605 K due to an increase in the carrier concentration, as evidenced by theoretical calculations using density functional theory (DFT). Additionally, the total thermal conductivity, κtotal, was significantly reduced from 2.26 to 0.83 W/mK at 605 K for the compositions of CuFeS2 and CuFeS1.8, respectively, owing to the enhanced phonon scattering from the strong acoustic phonon coupling, Umklapp process, and sulfur vacancy-driven low group velocity. Consequently, the sulfur-deficient CuFeS1.8 sample exhibited the highest thermoelectric figure of merit, zT, of 0.14 at 605 K with a notably high hardness of 158 Hv, proving that it is an efficient thermoelectric material for intermediate temperatures.	6.4	https://pubs.acs.org/doi/abs/10.1021/acsaem.3c03176	2024
Jayabrata Das,Sangya Bhattacharjee	ACS Applied Bio Materials	Electropotential-inspired star-shaped gold nanoconfined multiwalled carbon nanotubes: A proof-of-concept electrosensoring interface for lung metastasis biomarkers	Herein, an innovative way of designing a star-shaped gold nanoconfined multiwalled carbon nanotube-engineered sensoring interface (AuNS@MWCNT//GCE) is demonstrated for quantification of methionine (MTH); a proof of concept for lung metastasis. The customization of the AuNS@MWCNT is assisted by surface electrochemistry and thoroughly discussed using state-of-the-art analytical advances. Micrograph analysis proves the protrusion of nanotips on the surface of potentiostatically synthesized AuNPs and validates the hypothesis of Turkevich seed (AuNP)-mediated formation of AuNSs. In addition, a facile synthesis of electropotential-assisted transformation of MWCNTs to luminescent nitrogen-doped graphene quantum dots (Nd-GQDs avg. 4.3 nm) is unveiled. The sensor elucidates two dynamic responses as a function of CMTH ranging from 2 to 250 μM and from 250 to 3000 μM with a detection limit (DL) of 0.20 μM, and is robust to interferents except for tiny response of a similar −SH group bearing Cys (<9.00%). The high sensitivity (0.44 μA·μM–1·cm–2) and selectivity of the sensor can be attributed to the strong hybridization of the Au nanoparticle with the sp2 C atom of the MWCNTs, which makes them a powerful electron acceptor for Au–SH–MTH interaction as evidenced by density functional theory (DFT) calculations. The validation of the acceptable recovery of MTH in real serum and pharma samples by standard McCarthy–Sullivan assay reveals the holding of great promise to provide valuable information for early diagnosis as well as assessing the therapeutic consequence of lung metastasis.	4.7	https://doi.org/10.1021/acsabm.2c00605	2022

Vijay Srinivasan and Tushar H Rana	Physica Scripta	First principle insights into the physical properties of Ti-based 211-MAX phase nitrides Ti2AN (A=Tl and Pb)	We have used the theoretical ab initio approach to scrutinize the electronic and other physical properties of Ti2AN(A=Tl and Pb). Geometrical optimization has been carried out to obtain accurate lattice constants and internal coordinates. The formation energies of Ti2TlN and Ti2PbN are found to be negative, which confirms their stability. The aforementioned compounds are found to be metallic because of their zero-band gaps. The metallicity fm (x 10−3) of Ti2TlN and Ti2PbN phases were determined to be 1.77 and 2.11, respectively. In addition, we evaluate the elastic constant Cij, which obeys the Born-Huang mechanical stability criterion.Weused the Voigt-Reuss-Hill approximation for the analysis of Young’s modulus, shear modulus, and bulk modulus successfully. Furthermore, Ti2TlN is found to be brittle, but Ti2PbN is close to the brittle-ductile boundary line according to Pugh’s and Poisson’s ratios. The Debye temperature, melting temperature, and minimum thermal conductivity have all been rigorously studied to examine the potential scenarios of genuine high-temperature applications. Lower Young’s modulus, the minimum thermal conductivity (Ti2TlN and Ti2PbN), and Debye temperature values reveal that Ti2PbN might be used as a thermal barrier coating application. A study of elastic anisotropy demonstrates that Ti2PbN has a higher degree of anisotropy than Ti2TlN, according to the universal anisotropy index.Weconfirmed the dynamic stability (i.e., no negative frequencies at the gamma point) of predicted compounds by performing phonon DOSand phonon band structures. Finally, the temperature-dependent thermodynamic properties of Ti2TlN and Ti2PbN have been thoroughly analyzed, where the entropy (S), free energy, and internal energy (E) vary with respect to temperature. Moreover, the convergence of specific heat capacity is observed at constant volume to the Dulong-Petit limit at higher temperatures.	2.9	https://iopscience.iop.org/article/10.1088/1402-4896/acfffe/meta?casa_token=1iPG129z6eYAAAAA:E1rUFG4lk6jih5rTlvd7yuEDh8Itdg7JqoamUpTG7Ny9ix6e1akG4nPflCff1YkekJO4Biwypq8n8i_9wZ-QjjsAJlJN	2023
Sakthi Balaji A,R.Akash	Surfaces and Interfaces	Chemical Modification of Aluminum Nitride Nanotubes (AlNNT) using-OH, C= O, R-SH functional groups: First Principle's study	https://drive.google.com/file/d/1FuwKAqgfoXxx5G-Jq37K2ktS3GXLfHew/view?usp=sharing	6.2	https://www.sciencedirect.com/science/article/abs/pii/S2468023023006326	2023
Sakthi Balaji A,R.Akash	Surfaces and Interfaces	Covalent modification of single-walled boron nitride nanotube (BNNT) with amino acids: Ab initio method	https://drive.google.com/file/d/12bhaOxTOhvxkLPQnnK8Du4XxtOK_7DiF/view?usp=sharing	6.2	https://www.sciencedirect.com/science/article/abs/pii/S2468023023007071	2023
Sakthi Balaji A,R.Akash	ECS Journal of Solid State Science and Technology	Chemical functionalization of silicon carbide nanotube (SiCNT): First principles DFT study	https://drive.google.com/file/d/10XKsfx1_FJLx0XL7YmMUe-FdfI9Fzo3I/view?usp=drive_link	2.2	https://iopscience.iop.org/article/10.1149/2162-8777/ad0327/meta	2023

Sakthi Balaji A	Journal of Physics and Chemistry of Solids	First-Principles Studies on Tuning the Geometrical, Electronical, and Optical Traits of 2D α-GeTe/Sb Van der Waals Heterostructure		4		UNDER REVIEW
Sakthi Balaji A	ICONN Internatioanl Conference, SRMIST	Modulating the electronic and optical properties of 2D BuckledαGeTe Monolayer with point defects: A First principle study			https://drive.google.com/file/d/1zJaDKBhacAyASOOcLOLlOWkoibAUWBYe/view?usp=sharing	2023
Sakthi Balaji A	Raman 23 Natioanl Conference, DIT university	GEOMETRIC AND ELECTRONIC PROPERTIES OF 2D α GeTe/Sb VAN DER WAAL'S HETEROSTRUCTURE: A FIRST PRINCIPLES STUDY			https://drive.google.com/file/d/1HvzEwU87loXjioo35wzfNUDO3GGJMt5H/view?usp=sharing	2023
Sakthi Balaji A	AFMD 24, Internatioanl Conference, SRMIST	Structural and Electronic Properties of 2D GeTe/Arsenene vdW Heterostructure: A First-Principles Study			https://drive.google.com/file/d/10SULBgHUr9LjBRWXNRzvNSKNSMo7Ytbd/view?usp=sharing	2024
Poornimadevi C	ECS Journal of Solid State Science and Technology	Ab Initio Study of Electronic Properties on WS2 Monolayer and Transition Metal Doped WS2	-	2.2	Ab Initio Study of Electronic Properties on WS2 Monolayer and Transition Metal Doped WS2 - IOPscience	2022
Poornimadevi C	MaterialsScienceinSemiconductorProcessing	Tuning the electronic properties of WS2 monolayer by doping transition metals: DFT Approach	-	4.1	Tuning the electronic properties of WS2 monolayer by doping transition metals: DFT Approach - ScienceDirect	2023

Poornimadevi C	Surfaces and Interfaces	First principle analysis of toxic gas adsorption on pristine WS2 and Fe-doped WS2: Implications for gas sensing	-	6.2	[First principle analysis of toxic gas adsorption on pristine WS2 and Fe-doped WS2: Implications for gas sensing - ScienceDirect]()	2023
R.Akash	ECS Journal of Solid state science and Technology	Chemical Functionalization of Silicon Carbide Nanotube (SiCNT): First Principles DFT Study	In this study, a functionalized nano drug carrier design based on (5,5) silicon carbide nanotube and functional groups such as amine (−NH2), hydroxyl (−OH), and carboxylic acid (−COOH) were investigated using the first principles' density functional theory. The critical need for a smart nanocarrier system aims to increase the concentration of medications to the particular tissues of interest with minimal toxicity to the patient. The simulations are carried out using Quantum ATK-Atomistic Simulation Software. The negative binding energy and the total energy difference obtained by optimization through random perturbation ensure the stability of the structures SiCNT and SiCNT-(X/2X) (X = −OH, −NH2, and −COOH). The energy bandgap obtained for the pristine structure is 1.99 eV indicating their indirect bandgap semiconducting characteristics. In comparison to SiCNT, the energy bandgap of SiCNT-(X/2X) structures decreases within a range of 0.06 eV to 1.95 eV, respectively. Partial charges and p-character were used to understand the nature of bonds between the nanotube and the functional moiety. The chemical potential analysis favors a blue shift of SiCNT-(X/2X) with respect to SiCNT. The higher values of ionic character and solvation energy predicts the solubility of nanostructures in the aqueous medium. In comparison to all analyzed systems, the findings of the ionic character, solvation, and sensing mechanism indicate SiCNT-(2NH2) system to be most favorable drug delivery nanocarrier. These findings suggest that increasing the concentration of −NH2 functional groups on the side wall of silicon carbide nanotubes helps to develop a promising and efficient targeted drug delivery system to deliver specific molecular cargo to the cells mitigating toxicity associated with nanotubes, thereby enhancing the outcomes of cancer treatment. Furthermore, surface functionalization of silicon carbide nanostructures could improve their potential solubility parameterized by higher values of dipole moment and solvation energy together with enhanced biocompatibility leading to the desired therapeutic effect.	2.2	https://iopscience.iop.org/article/10.1149/2162-8777/ad0327/meta	2023

R.Akash	ICONN-2023,SRMIST,Kattankulathur	VOCs adsorption on defect induced and doped armchair silicene nanoribbon: Ab initio method	Silicene has emerged as a potential few-atom-thick material to replace graphene. Theoretical investigations noted that like graphene, silicene is a semimetal with a Dirac cone and a zero electronic band gap. Cutting silicene along one axis produces quasi-one-dimensional silicene nanoribbons (SiNRs). Based on edge orientation, SiNRs are classified as armchair silicene nanoribbons (ASiNRs) and zigzag silicene nanoribbons (ZSiNRs). ZSiNR is also semimetal with zero bandgap but, ASiNR has semiconducting nature and width dependent bandgap. In this work, we studied the stability and electronic properties of pristine armchair silicene nanoribbon (ASiNR), single vacancy induced ASiNR (D-ASiNR), B, C, and N doped ASiNR(B, C, and N ASiNR). Formation energy was calculated to prove the stability, and from this C and N-ASiNR shows better stability than any other systems, and D-ASiNR showed poor stability. The electronic properties like bandstructure, DOS, and PDOS were calculated. B and N-ASiNR have zero bandgap other systems have semiconducting nature. Then adsorption of VOCs (Isoprene) which is used as a breath biomarker, in all the systems was studied. Further to understand the sensing behaviour, adsorption energy, adsorption distance, charge transfer, and electronic properties were calculated. Our findings suggested that doped and defect induced systems exhibit higher sensitivity toward VOCs	Poster presented	https://drive.google.com/file/d/1oIn6gHfsZ4YJtutzhTArG3DTwSXHc49I/view?usp=drive_link	2023
R.Akash	RAMAN-2023,DIT University, Dehradun	FIRST PRINCIPLES INSIGHT ON B AND N-DOPED ARMCHAIR SILICENE NANORIBBON FOR LUNG CANCER BREATH BIOMARKER DETECTION	Lung cancer (LC) is one of the leading causes of cancer deaths in the world. Early detection of LC can be helpful to reduce the mortality rate of cancer deaths. The easiest and most cost-effective method is the breath analysis of humans. Human breath contains volatile organic compounds (VOCs) that act as a biomarker. Isoprene is recognized as an LC breath biomarker and sensing the isoprene will be helpful in the diagnosis of LC. In this work, Density functional theory (DFT) was carried out to study the structural and electronic properties of armchair silicene nanoribbon (ASiNR), B, and N-doped ASiNR systems. The structural stability was studied by binding energy values and the N-doped ASiNR system shows good stability. The electronic properties like bandstructure and density of states were calculated. The pure ASiNR system has semiconducting nature, B and N- doped ASiNR system has zero band gap. Then we studied the adsorption behaviour of isoprene towards all the systems by calculating the adsorption energy, adsorption distance, and charge transfer. For further understanding of the adsorption mechanism, we study the electronic properties. Our results exploit ASiNR can be a good sensor for LC biomarker.	Poster presented	https://drive.google.com/file/d/12j50itiVq9Sizh_LQ3SGZpqktRGoU2rK/view?usp=drive_link	2023

R.Akash	AFMD-2024,SRMIST,Kattankulathur	DFT investigation on sensing the VOCs on mono and di-vacancy induced armchair silicene nanoribbon	Volatile organic compounds (VOCs) play a vital role in the early detection of diseases. More than 200 VOCs are released in human breath and few of them are used as a biomarker. These kinds of VOCs are released due to the metabolic changes in the human body. VOC detection is a quick, noninvasive, and cost-effective method for early detection of many diseases. Nanomaterial-based sensors are efficient for sensing the VOCs with high selectivity and sensitivity. Among the class of materials, xenes are compatible materials for sensing the VOCs due to the high surface to-volume ratio, high surface reactivity, and excellent electron mobility. Apart from graphene, silicene attracts many researchers due to its low-buckling nature from the xenes group. Silicene nanosheets pose a semi-metallic nature similar (a) (b) (c) (d) to graphene which makes this material lack tunable properties. But armchair silicene nanoribbons (ASiNR) have semi conducting behavior with tunable electronic properties also widely reported for sensing applications. This makes this material for sensing the VOCs in the exhaled breath. In the present work, we are using the DFT approach to study the ground-state electronic properties and structural properties of pure ASiNR, mono and divacancy-induced ASiNR. Then we studied the adsorption behavior of colorectal cancer breath biomarkers cyclohexane(C6H12), methylcyclohexane(C6H11CH3), and 1,2-pentadiene(C5H8) towards all the systems. The structural stability of the system is confirmed through the formation energy. Then the adsorption energy, adsorption distance, charge transfer, and recovery time are also calculated. These results would give some insights into making a VOC sensor for the early diagnosis of diseases	Poster presented	https://drive.google.com/file/d/1UxSBo5GBtTBBZIGuvg4HNyvq3yE7bEFV/view?usp=drive_link	2024
R.Akash	ECS Journal of Solid state science and Technology	DFT calculations on Defect induced and doped ASiNR for sensing the COPD breath Biomarker	Cardiac Obstructive Pulmonary Disease (COPD) is one of the respiratory diseases with a high mortality rate worldwide. The major cause of death in COPD patients is due to late diagnosis. Early detection of COPD is crucial for significantly reducing the risk of death but is challenging to attain. A distinguished way to early diagnosis is by using the nanosensor for sensing the COPD breath biomarkers. For the first time, we report an armchair silicene nanoribbon (ASiNR) as a sensing material for the diagnosis of hexanal a promising COPD breath biomarker. In this study, the Density functional theory (DFT) approach was incorporated to observe the adsorption behaviour of hexanal on the pristine ASiNR system. To enhance the sensitivity, we introduced defect (D) and doping (B, C, N atoms) in ASiNR systems. The structural stability was analysed through the formation energy, C and N-doped ASiNR systems exhibit the highest stability. The adsorption energy was calculated for all the hexanal adsorbed systems. N-ASiNR systems show the highest adsorption energy value compared to previous literature which is due to the presence of strong covalent interaction, and it does not show recovery at room temperature. Whereas the B-ASiNR system has a huge amount of charge transfer with hexanal which causes a large amount of change in the work function. Also, the fastest recovery at room temperature is 1.81 s. Electronic properties were also examined for further understanding of the adsorption of hexanal. Our results indicate B-doped ASiNR system acts as an efficient reusable work function-based sensor for the early diagnosis of COPD at room temperature.	2.2(manuscript submitted)		2024
Abinaya.V	Surface and interfaces/ICONN 2023	Chemical Modification of Aluminum Nitride Nanotubes (AlNNT) using-OH, C=O, R-SH functional groups: First Principle’s study		6.2	https://drive.google.com/file/d/1J8gZhqmeNDT5HWCpf8d47jfvTrMzov12/view?usp=drive_link	2023

D. Siva Krisna Reddy	Journal of Physics: Conference Series	Numerical simulations over a three-body launch vehicle for incompressible flows		Performed simulations helped in getting sponsered project from VSSC ISRO	https://iopscience.iop.org/article/10.1088/1742-6596/2054/1/012039/meta	, 25th October, 2021
D. Siva Krisna Reddy	Journal of Physics: Conference Series	Prediction of Drag Coefficient of a Base Bleed Artillery Projectile at Supersonic Mach Number		Performed simulations helped in getting sponsered project from VSSC ISRO	https://iopscience.iop.org/article/10.1088/1742-6596/2054/1/012013	, 25th October, 2021
D. Siva Krisna Reddy	Journal of Physics: Conference Series	Computation of Three-Dimensional Transonic Flow fields over a three-body launch Vehicle Configuration for Low Angle of Attack Conditions		Performed simulations helped in getting sponsered project from VSSC ISRO	https://iopscience.iop.org/article/10.1088/1742-6596/2054/1/012012	, 25th October, 2021
Dr Susnata Pramanik	Chemical Communications	Excitation wavelength-dependent multi-coloured and white-light emissive pyrene-based hydrazones: suppression of Kasha's rule	Multi-coloured and white-light emissions from pyrene-based hydrazones are described. They exhibit excitation wavelength-dependent emissions in solution due to the suppression of Kasha's rule. Interestingly, in dimethylformamide, 1–3 emit light that covers all the regions of primary colours as a function of excitation wavelength, and 1 and 2 emit white light (λ_{ex} = 420 nm) in isopropanol.	4.9	https://pubs.rsc.org/en/content/articlelanding/2023/cc/d3cc04584f	2023
Dr Susnata Pramanik	New Journal of Chemistry	The effect of substituents on the aggregation-induced emission of 9,10-phenanthraquinone-hydrazones	Organic luminophores, particularly π-conjugated systems, have become crucial in modern optoelectronic devices that utilise luminescence as an output signal, requiring aggregate or solid-states, such as nanoparticles, thin films, or crystals. Herein, we report the one-step synthesis of six hydrazone derivatives using condensation reactions between 9,10-phenanthrenedione and different aromatic hydrazines, comprising electron-donating/electron-withdrawing groups and a quinoline moiety. The introduction of a conjugated π-system leads to complete co-planarization of molecules resulting in large bathochromic shifts in their absorption profile, the maximum red-shifts ever observed for the hydrazones. These hydrazones are weakly fluorescent in dilute acetonitrile solutions. However, they exhibit enhanced emissions of up to 300-fold in aggregated states. Dynamic light scattering (DLS) and scanning electron microscopy (SEM) studies support nanoaggregate formation. All the compounds exhibit red to NIR emissions in their crystalline state with as high as 75% quantum efficiency.	3.6	https://pubs.rsc.org/en/content/articlelanding/2023/nj/d3nj02198j	2023
Sneha.J	Surface and interfaces/ICONN2023	Covalent Modification of Single-Walled Boron Nitride Nanotube(BNNT) with amino acids:AB initio method		6.2	https://drive.google.com/file/d/1yrr4eTkXLYUJfckl2pHS6HyAFxbz8C3U/view?usp=drive_link	2023

S. Iyappan	Journal of applied biology and biotechnology	Identification of noval non-coding RNAs in Rhizoctonia solani through mining of transcriptomic data. Journal of applied biology and biotechnology	Rhizoctonia solani is a plant pathogenic fungus infecting a wide range of hosts including economically important crops such as wheat, rice, and vegetables, etc. and leads to a loss in agricultural production. Various chemicals and bio fungicides are used to control R. solani. Understanding of gene expression and its function during host interaction will be useful to identify potential targets in R.solani for its effective control. In recent studies, non-coding RNAs (ncRNAs) are found to have a role in regulating cellular functions. In the current study, we report 16 ncRNAs from R. solani identified using raw transcriptomic data from three different bio projects reported in NCBI's sequence read archive database. The ncRNAs from F001 to ncRNA F0011 was expressed with fragments per kilo million reads (FPKM) values ranging from 100 to 20,000. Out of these 11 ncRNAs, 7 ncRNAs has the same intron splicing sites in all three bio projects. The ncRNA F0012 to ncRNA F0016 was found to be expressed approximately 10–80 FPKM and are present in all three bio projects, out of these five ncRNAs, three are found to have similar splicing sites in all three bio projects. The high expression levels of the ncRNAs and their presence in the genome confirmed by different datasets point to the fact that they might have a major function in the organism and should be studied further to characterize it functionally and the current study might serve as the first step to achieve it.	Journal Publication	https://jabonline.in/admin/php/uploads/643_pdf.pdf	2021
S. Iyappan	Microbiological Research	Genomic characterization of Enterobacter xiangfangensis STP-3: Application to real time petroleum oil sludge bioremediation	Sustainable treatment of petroleum oil sludge still remains as a major challenge to petroleum refineries. Bioremediation is the promising technology involving bacteria for simultaneous production of biosurfactant and followed by degradation of petroleum compounds. Complete genomic knowledge on such potential microbes could accentuate its successful exploitation. The present study discusses the genomic characteristics of novel biosurfactant producing petrophilic/ petroleum hydrocarbon degrading strain, Enterobacter xiangfangensis STP-3, isolated from petroleum refinery oil sludge contaminated soil. The genome has 4,584,462 bp and 4372 protein coding sequences. Functional analysis using the RAST and KEGG databases revealed the presence of biosynthetic gene clusters linked to glycolipid and lipopeptide production and multiple key candidate genes linked with the degradation pathway of petroleum hydrocarbons. Orthology study revealed diversity in gene clusters associated to membrane transport, carbohydrate, amino acid metabolism, virulence and defence mechanisms, and nucleoside and nucleotide synthesis. The comparative analysis with 27 other genomes predicted that the core genome contributes to its inherent bioremediation potential, whereas the accessory genome influences its environmental adaptability in unconventional environmental conditions. Further, experimental results showed that E. xiangfangensis STP-3 was able to degrade PHCs by 82 % in 14 days during the bioremediation of real time petroleum oil sludge with the concomitant production of biosurfactant and metabolic enzymes, To the best of our knowledge, no comprehensive genomic study has been previously reported on the biotechnological prospective of this species	Journal Publication	https://www.sciencedirect.com/science/article/pii/S0944501321001889	2021

Meera M Nair	ernational Journal of Climatol	Quantification of uncertainties in projections of extreme daily precipitation simulated by CMIP6 GCMs over homogeneous regions of India	PublishedGlobal climate model (GCM) projections are subject to significant uncertainties. Quantifying uncertainties in climate change projections improves credibility and makes climate data more reliable. This study aims to quantify the uncertainties in projected extreme precipitation during the 21st century over the homogeneous rainfall regions of India simulated by Coupled Model Intercomparison Project – phase 6(CMIP6) GCMs. The percentile-based square root error variance (SREV) method estimates model, scenario, and ensemble uncertainties in projections of extreme precipitation. The uncertainty is investigated at four thresholds, 95th, 99th, 99.9th, and 100th percentiles. The results show that the wet northeast region has a greater SREV, which is consistent with previous studies. At 99th and 99.9th percentiles, relative model SREV is dominant over the northeast region. However, at the 95th percentile high relative model SREV is found over the northwest region during southwest (June, July, August, and September) and northeast (October, November, and December) monsoon seasons. Model uncertainty is the main source of uncertainty, followed by scenario and ensemble uncertainties. The study indicates that the arid northwest region in India has a higher level of uncertainty than other regions with homogeneous rainfall. These findings will assist policymakers in planning infrastructure development in arid regions of India.	3.61	0.1002/joc.826	2023
T.Kesavavarthini	International Journal of Climatology	Bias Correction of CMIP6 Simulations of Precipitation over Indian Monsoon Core Region using Deep Learning Algorithms	General Circulation Models or Global Climate Models (GCMs) output consists of inevitable bias due to insufficient knowledge about parameterization schemes and other mathematical computations that involve thermodynamical and physical laws while designing climate models. Indian summer monsoon (southwest monsoon) accounts for 75 to 90% of the annual rainfall over most climatic zones of India during the months, June, July, August, and September, which has a direct impact on the agricultural economy of India. The aim of this study is to bias correct the Coupled Model Intercomparison Project Phase – 6 (CMIP6) GCMs' precipitation data for the historical period from 1985 to 2014 and two Shared Socioeconomic Pathways (SSP) SSP1-2.6 and SSP5-8.5, from the period 2015 to 2100, with reference to the India Meteorological Department (IMD) observed rainfall gridded dataset. The datasets used are for the rain-bearing Indian southwest monsoon season from the months, June to September. Monsoon Core Region (MCR) is selected to carry out the bias correction using a couple of deep learning algorithms, namely one-dimensional Convolutional Neural Network (CNN1D) and Long Short-Term Memory Encoder-Decoder (LSTM-ED) Neural Network. The performance of both algorithms is evaluated with metrics. The LSTM-ED algorithm yielded better results with least error output. The bias corrected data obtained using the LSTM-ED algorithm is then compared with IMD observed rainfall data for the climatic events such as ENSO (El Niño and La Niña) and Positive and Negative IOD (Indian Ocean Dipole).	3.6	https://rmets.onlinelibrary.wiley.com/doi/10.1002/joc.8056	2023

A.Sabarinath	International Journal of Climatology	Application of deep learning algorithms to correct bias in CMIP6 simulations of surface air temperature over the Indian monsoon core region	Indian subcontinent witnessed a rise in surface air temperature (SAT) in recent decades, during the summer months of March, April and May. The monsoon core region (MCR) of India experiences a hot and humid climate, with temperatures typically highest in May and June before the onset of the monsoon. Global climate model (GCM) simulations of SAT are very much essential to understand the future climate of Indian MCR. Biases in GCMs simulations are due to insufficient knowledge of parameterizations and various assumptions that are made to simulate the complex interactions between land, ocean and atmosphere. The objective of this study is to correct the bias in the Coupled Model Intercomparison Project Phase 6 (CMIP6)–GCM simulations of SAT during March, April and May months over MCR for the historical period 1985–2014 and shared socio-economic pathways (SSPs) SSP2-4.5 and SSP5-8.5 for the period 2015–2100. SAT dataset of fifth-generation reanalysis (ERA5) of the European Centre for Medium-Range Weather Forecasts (ECMWF) is used as reference dataset to perform bias correction for the historical period. Preliminary investigation of both SAT datasets has shown that there exists considerable warm bias (1.47°C) over the MCR. Bias correction is performed using a one-dimensional convolutional neural network (CNN-1D) and a convolutional long short-term memory network (CNN-LSTM) deep learning algorithm. The performance of these algorithms is evaluated with the statistical metrics such as root-mean-square error (RMSE), normalized root-mean-square error, Nash–Sutcliffe efficiency, mean absolute error, percent bias, correlation coefficient and dynamic time warping. RMSE and percent bias were decreased to 0.35°C and 0.8% with CNN-LSTM algorithm. The CNN-LSTM algorithm also preserves the year-to-year variability of SAT. Hence, CNN-LSTM algorithm is found to be suitable for the bias correction of GCM simulations of SAT with encouraging results.	3.61	https://doi.org/10.1002/joc.8276	2023
Gokul, G., Malaikannan, G.	AIP Conference Proceedings	The Chemically Reacting Hypersonic Flow over a Reentry Capsule with Hybrid Chemical Reaction Models			https://pubs.aip.org/aip/acp/article-abstract/2996/1/150004/3262736/The-chemically-reacting-hypersonic-flow-over-a?redirectedFrom=fulltext	2024
Murtuzapurwala, N., Malaikannan, G.	The Proceedings of the Institution of Mechanical Engineers, Part G: Journal of Aerospace Engineering	Thermo-chemical and Structural Analysis of Integrated Thermal Protection System for a Space Vehicle			https://journals.sagepub.com/doi/10.1177/09544100231206568?icid=int.sj-abstract.similar-articles.4	2023
Sharma, S., Sharma, H., Ansari, H., Malaikannan, G.	Journal of Thermophysics and Aeromechanics	Aerothermodynamic Design Optimization of Planetary Vehicle			https://link.springer.com/article/10.1134/S0869864323030046	2023

Ravi Gor, Ali Gharib,Priya Dharshini Balaji,Thirumurthy Madhavan and Satish Ramalingam*	Toxics	Inducing Cytotoxicity in Colon Cancer Cells and Suppressing Cancer Stem Cells by Dolasetron and Ketoprofen through Inhibition of RNA Binding Protein PUM1	Clinical trials of new drugs often face a high failure rate of approximately 45 percent due to safety and toxicity concerns. Repurposing drugs with well-established safety profiles becomes crucial in addressing this challenge. Colon cancer ranks as the third most prevalent cancer and the second leading cause of cancer related mortality worldwide. This study focuses on the RNA-binding protein pumilio1 (PUM1), a member of the PUF family involved in post-transcriptional gene expression regulation. By utilizing molecular docking techniques and FDA-approved drugs, potential inhibitors against PUM1 were identified. Notably, dolasetron and ketoprofen demonstrated promising results, exhibiting strong binding affinity, hydrophobic interactions, and favorable chemical reactivity according to Conceptual-DFT calculations. Both compounds effectively reduced cell viability, with IC50 values of 150 µM and 175 µM, respectively and shows long term inhibitory effects as seen by reduced in number of colonies. Moreover, they exhibited inhibitory effects on colon cancer stem cells, as indicated by reduced colonospheroid size and numbers. Apoptosis is induced by these compounds and has triggered activation of executioner caspase 3/7 in HCT116 cells which is evident through a caspase 3/7 assay and AO/EB staining, while the non-toxic effect of these compounds was evident from viability against non-cancerous cell line and hemolysis assay. Additionally, the treatment group showed a significant decrease in PUM1 and cancer stem cell markers expression compared to the control group. In conclusion, this study highlights the potential of targeting PUM1 as a novel approach to colon cancer treatment. Dolasetron and ketoprofen demonstrate promise as effective anti-cancer and anti-cancer stem cell drugs, inducing apoptosis in colon cancer cells through inhibition of PUM1.	4.6	https://www.mdpi.com/2305-6304/11/8/669	2023
T Sahoo	Journal of Physical Chemistry	First-Principles Study of Fe	Organic ferroelectric materials in the form ofmolecular crystals are promising alternatives to	3.7	https://pubs.a	2022
T Sahoo	Optical Materials	Growth and characterizati	A new organic material of 2-Methylbenzimidazole 4-Aminobenzoate (2MIAB) with a size of 5	3.75	https://www.sciencedirect.com/science/article/abs/pii/S0925346723013411?via%3Dihub	2024

Arunmozhi Bharathi Achudhan	Frontiers in Molecular Bioscience	Functional metagenomics uncovers nitrile-hydrolysing enzymes in a coal metagenome	Nitrilases can highly degrade nitriles isolated from the natural ecosystem. In the current study, we focused on the discovery of novel nitrilases from a coal metagenome using in silico mining. Coal metagenomic DNA was isolated and sequenced on the Illumina platform. Quality reads were assembled using MEGAHIT, and statistics were checked using QUAST. Annotation was performed using the automated tool SqueezeMeta. The annotated amino acid sequences were mined for nitrilase from the unclassified organism. Sequence alignment and phylogenetic analyses were carried out using ClustalW and MEGA11. Conserved regions of the amino acid sequences were identified using InterProScan and NCBI-CDD servers. Furthermore, NetSurfP was used for 2D structure prediction, while AlphaFold2 in Chimera X 1.4 was used for 3D structure prediction. To check the solvation of the predicted protein, a dynamic simulation was conducted on the WebGRO server. Ligands were extracted from the Protein Data Bank (PDB) for molecular docking upon active site prediction using the CASTp server. In silico mining of annotated metagenomic data revealed nitrilase from unclassified Alphaproteobacteria. By using the artificial intelligence program AlphaFold2, the 3D structure was predicted with a per-residue confidence statistic score of about 95.8%, and the stability of the predicted model was verified with molecular dynamics for a 100-ns simulation. Molecular docking analysis determined the binding affinity of a novel nitrilase with nitriles. The binding scores produced by the novel nitrilase were approximately similar to those of the other prokaryotic nitrilase crystal structures, with a deviation of ±0.5.	5	https://www.frontiersin.org/articles/10.3389/fmolb.2023.1123902/full	2023
Arunmozhi Bharathi Achudhan	Functional & Integrative Genomics	CRISPR detection in metagenome-assembled genomes (MAGs) of coal mine	Bacterial and archaeal CRISPR-Cas systems provide adaptive immune protection against foreign mobile genetic elements. When viruses infect bacteria, a small portion of the viral DNA is inserted into the bacterial DNA in a specific pattern to produce segments known as CRISPR arrays. Metagenome assembled genomes (MAGs) were used in our study to identify the CRISPR sequence for determining the interacted phage. Metagenomic data from a coal mine was used to perform a computational study. From raw reads, 206151 contigs were assembled. Then contigs were clustered into 150 Metagenome assembled genomes from which 78 non-redundant MAGs were selected. Using the CHECKM standard, seven MAGs were found to have >80 completeness and <20 contaminations. Those MAGs were analyzed for the presence of CRISPR elements. Out of seven MAGs, four MAGs have the CRISPR elements and are searched against the VIROblast database. CRISPR arrays have 4, 1, 3, and 7 spacer sequences in the MAGs of Burkholderia, Acinetobacter, Oxalobacteraceae, and Burkholderia multivorans respectively. The uncultured Caudovirales phage genomic regions were present in the genomes of Burkholderia, Oxalobacteriaceae, and Burkholderia multivorans. This study follows the unconventional metagenomics workflow to provide a better understanding of bacteria and phage interactions.	2.9	https://pubmed.ncbi.nlm.nih.gov/37043060/#:~:text=When%20viruses%20infect%20bacteria%2C%20a,for%20determining%20the%20interacted%20phage.	2023

Priya Kannan	Archives of Microbiology	Unveiling bacterial consortium for xenobiotic biodegradation from Pichavaram mangrove forest soil: a metagenomic approach	Pichavaram mangrove forest was established as a wetland of International Importance by Article 2.1 in April 2022 by the Ministry of Environment, Forest and Climate Change, India. Even though it is a conserved site, xenobiotic agrochemical leaching on the forest land during monsoon is inevitable. These threaten the microbial diversity in the environment. Xenobiotic degradation is achieved using bacterial consortia already acclimatised to this environment. This study aims to identify the indigenous microbial consortia able to degrade xenobiotic compounds such as fluorobenzoate, furfural, and steroids. Pichavaram mangrove metagenomic dataset was obtained by shotgun sequencing of soil DNA and processed using the automated tool SqueezeMeta. Further, the DIAMOND database provided the taxonomical classification of the microbes in each contig. With reference to the KEGG database, the selected xenobiotic degradation pathways were confirmed in the dataset. Of 1,253,029 total contigs, 1332, 72 and 1262 were involved in fluorobenzoate, furfural and steroid degradation, respectively. This study identified that microbial consortia comprising Marinobacter, Methyloceanibacter and Vibrio natriegens/Gramella sp. can degrade fluorobenzoate. While Afipia, Nitrosopumilus sp., and Phototrophicus methaneseepsis favour the degradation of furfural compound. The steroid degradation pathway possessed a plethora of bacteria belonging to the phylum Proteobacteria.	2.8	https://link.springer.com/article/10.1007/s00203-023-03765-9	2023
J Preetha Roselyn	Computers, Materials and Continua, Tech science Press	Feature extraction and classification of photovoltaic panels based on convolutional neural network		SCI INDEX		2023
J Preetha Roselyn	Computers and Electrical Engineering	Development and Real Time Implementation of Intelligent Holistic Power Control for Stand Alone Solar Photovoltaic Generation System		SCI INDEX		2021
J Preetha Roselyn	Expert systems with applications	Anomaly Detection in Multivariate Streaming PMU Data using Density Estimation Technique in Wide Area Monitoring System		SCI INDEX		2021

Dr. Prakash Muthuramalingam	Crystal Growth & Design	Tuning Diffusion Permeability of an Anti-Retroviral Drug Emtricitabine, via Multicomponent Crystallizations.	Emtricitabine (ECB) is an anti-retroviral drug that inhibits HIV reverse transcriptase and prevents transcription of RNA to DNA. ECB exhibits high solubility and low permeability (log P < 0). To modify the diffusion behavior of ECB, a high throughput cocrystal screening has been carried out with coformers that contain carboxylic acid/amide functionalities via solvent assisted grinding. The screening study resulted in the formation of cocrystals with benzoic acid (BA), caprolactam (CPR), and salts with 2,6-dihydroxybenzoic acid (DHBA), malonic acid (MLN), maleic acid (MLE), and saccharin (SAC), which were confirmed with single crystal X-ray diffraction. In addition, 15N solid state NMR spectroscopy was exploited to define the ionization state of the multicomponent systems. The 2-aminopyrimidine homodimer of the cytosine analogue in the ECB is replaced by aminopyrimidine···carboxylic acid/amide in the cocrystals and aminopyrimidinium···carboxylate/saccharinate heterosynthons in the salts. The terminal hydroxyl group of the ECB forms a hydrogen bond with its carbonyl group, which is consistent in the ECB–BA cocrystal, ECB–DHBA and ECB–MLN salts. In addition, the hydroxyl group of ECB is hydrogen bonded with the relatively stronger acceptors like the carbonyl/sulfonyl group of caprolactam, maleate, and saccharinate in their corresponding multicomponent crystals. The diffusion studies of ECB multicomponent crystals using a Franz diffusion cell suggest that the ECB–BA cocrystal exhibited an enhanced diffusion and flux compared to that of native drug and other multicomponent crystals. An inverse correlation was observed partially between the flux values with crystal densities and binding energies of the ECB multicomponent systems.	3.8	https://pubs.acs.org/doi/abs/10.1021/acs.cgd.0c01344	2021
Dr. Prakash Muthuramalingam	Solar Energy	Incorporation of organic additives with electron rich donors (N, O, S) in gelatin gel polymer electrolyte for dye sensitized solar cells	A new sequence of GLN gel polymer electrolytes incorporated with KI/I2 redox pair and inexpensive organic additives were prepared. Five dissimilar N, O, and S containing organic compounds were used as additives for the application of DSSCs. The assimilation of organic additives into the GLN gel polymer electrolytes is confirmed by FTIR, DSC, XRD, UV–visible and SEM analyses. EIS analysis reveals that there is an increment in the conductivity up to 2.93X10-5 S/cm for SAA organic additive integrated gel polymer electrolyte than other organic additives. This is owing to more electrons donating nature of the SAA molecule which consists of N, S and O atoms together in its structure. The EIS experiment exposes the interfacial study in DSSCs to elucidate the charge transport mechanisms at the interface of photo electrodes and electrolyte medium of the devices. The charge transfer studies show a lower Rpt (685 Ω), higher Rct (1674 Ω) and Cμ (5.702 X 10-6F) values for SAA integrated GLN gel polymer electrolyte. This confirms mitigation of recombination process between TiO2 and I3- ions and also build a shift to Fermi level of TiO2. DFT calculations also confirm the strength and mode of interaction of individual additives adsorbed on TiO2 surfaces. The FMO analysis clearly reveals that functional groups play a vital role in the charge transfer process at interface materials. The N, O and S present in the SAA additive with GLN gel polymer electrolyte improves the PCE up to 5.8% under the sunlight illumination of 100mWcm−2.	6.7	https://www.sciencedirect.com/science/article/abs/pii/S0038092X21001870	2021

Dr. Prakash Muthuramalingam	Materials Science and Engineering B: Solid-State Materials for Advanced Technology	Vanadium silicon-oxyfluoride nanowires for lithium storage systems: A perfect synergy for dynamic simple spot synthesis	Polyanionic vanadium silicon oxyfluoride, LiVSiO4F (VSF) nanowire synthesize through a dynamic simple spot method exposes a multi-redox behavior with excellent reversibility and minimal capacity fade as electrodes in Li-ion systems. However, the cycling performance of the electrode is under debate due to its conductivity and polyanionic nature. To address this, an increase in the ratio of a conductive agent like 10%, 20%, and 30% is intermixed with cathodes, and as a result, the cathodes reveal an increasing electrochemical performance for VSF 30%. At a high current rate of 1Ag−1, VSF 20% and 30% express a specific capacity of 164 mAhg−1 and 230 mAhg−1 respectively, which is higher than the theoretical capacity. This is due to the anionic redox nature of O and F, apart from transition metal vanadium. VSF 30% exhibits a higher power density of 300Wkg−1 with an energy density of 623WhKg−1 that can be applicable in high-power devices.	3.4	https://khu.elsevierpure.com/en/publications/vanadium-silicon-oxyfluoride-nanowires-for-lithium-storage-system	2021
Dr. Prakash Muthuramalingam	The Journal of Physical Chemistry C	Enhancement of Second-Order Nonlinear Optical Properties of Centrosymmetric Ferrocenyl Borasiloxane by a Broken-Symmetry Approach	A new eight-membered centrosymmetric ferrocenyl borasiloxane FcBSi (1) and its pyridine adduct FcBSiPy (2) were synthesized and spectroscopically characterized. Further, the compound FcBSi (1) is confirmed by single-crystal X-ray diffraction studies, which crystallizes the triclinic crystal system in the centrosymmetric space group P1¯ with an eight-membered ring (B2O4Si2) configuration. Both the compounds FcBSi (1) and FcBSiPy (2) exhibit a negative solvatochromism in nonpolar to polar solvents because the dipole interactions between solvent and solute molecules make high ground-state dipole moments. The time-dependent density functional theory (DFT) calculations further support the same trend with the experimental results. Second-order nonlinear optical (NLO) properties of FcBSi (1) and its four coordinated pyridine adduct FcBSiPy (2) were studied by the Kurtz and Perry powder technique. The enhanced second harmonic generation efficiency (1.88 times) and ground-state dipole moment in 2 were achieved by breaking the symmetry through the formation of four coordinated boron pyridine adduct in the solid state. Further, optical and NLO properties were supported by DFT, which revealed enhanced polarizability (α0), hyperpolarizability (β0), and dipole moment (μtot) in FcBSiPy (2). © 2021 American Chemical Society. All rights reserved.	3.7	https://research.vit.ac.in/publication/enhancement-of-second-order-nonlinear-optical-properties	2021
Dr. Prakash Muthuramalingam	Biosensors and Bioelectronics	Novel SeS2-loaded Co MOF with Au@PANI Comprised Electroanalytical Molecularly Imprinted Polymer-based Disposable Sensor for Patulin Mycotoxin		12.6	https://pubmed.ncbi.nlm.nih.gov/34000454/	2021
Dr. Prakash Muthuramalingam	RSC Advances	Sodium ion intercalation and multi redox behavior of a Keggin type polyoxometalate during [PMo10V2O40]5− to [PMo10V2O40]27− as a cathode material for Na-ion rechargeable batteries	Recently, the development of cathode materials for Na-ion batteries has gained much attention due to the abundance, low cost, and easy availability of resources. Apart from the usual metal oxides, multi-electron redox materials grabbed attention due to their high energy density and practical capacity with long cycle life. Polyoxometalates (POMs) are inorganic clusters of higher valent metals, and act as electron sponges with multi-electron redox properties. Herein we report a Keggin-type polyoxometalate [PMo10V2O40]5− with Na+ and H+ counter cations as a cathode material for Na-ion batteries. Further the formation of POM is evidenced by PXRD, FT-IR, flame photometry and XPS studies. In Na-POM, Na+ ions in the intercluster cavities provide a better pathway and easy diffusion during the charge/discharge process, and contribute to better electrochemical properties than H-POM. The DFT studies further explore the detailed mechanistic pathway of Na+ ions around the clusters in the normal and super-reduced states. Na-POM enables better cycling stability and capacity retention with a specific discharge capacity of 123 mA h g−1 at 0.1C rate at room temperature.	3.9	https://pubs.rsc.org/en/content/articlelanding/2021/ra/d1ra02092g	2021

Dr. Prakash Muthuramalingam	Applied Surface Science	Ionic liquid incorporation in zeolitic imidazolate framework-3 for improved CO2 separation: A computational approach	Selective adsorption of gases from various mixtures of industrial importance has become a major concern. Improving the selectivity of the existing material by chemical/physical modification can solve this problem to an extent. In this regard, we incorporated ILs into the pores of well-known porous material, zeolitic imidazolate framework (ZIF). ZIF-3 has shown good selectivity for CO2 but their modification with ionic liquid (IL) has not yet explored. We studied 1-butyl-3-methylimidazolium ([BMIM]+) cation with seven different anions inside the confinement of ZIF-3 and their effect on the separation of CO2. Different orientations are checked and the stable one is selected for advanced computational studies. Pristine ZIF-3 and IL impregnated ZIF-3 shows good adsorption potential for CO2. The incorporation of ILs in ZIF-3 significantly enhances the CO2 capture from CO2/N2 and CO2/CH4 gaseous mixture. Whereas it is interesting that the adsorption of methane from CH4/N2 highly depends on the nature of IL (i.e. anion) inside the ZIF-3. Adsorption energies and heat of adsorption gives the strength of interaction between ILs, ZIF-3 and guest gaseous molecules. The ILs@ZIF-3 composites can perform better than well-known IL@ZIF-8 composite at higher pressure. The investigation of IL incorporation to various ZIFs can offer better CO2 selective material than the existing ones in the near future. Our combined density functional theory (DFT) and grand canonical Monte Carlo (GCMC) simulations are used to get more insights on the interfacial interactions between the ILs-ZIF structures and how these molecular level interactions can be helpful in the gas sensor applications and industrial flue gas separations.	6.7	https://www.sciencedirect.com/science/article/abs/pii/S0169433221012496	2021
Dr. Prakash Muthuramalingam	Materials Letters	Effect of functional group in the zeolitic imidazolate framework for selective CH4/CO and CO/N2 separation: A theoretical study	Zeolitic Imidazolate Frameworks (ZIFs), which is a sub-class of MOF has been evolving as a potential candidate in adsorption, storage and separation of environmental hazardous gases. In this work, ZIF-68 and ZIF-69 structures were analyzed using Grand Canonical Monte Carlo (GCMC) simulations for their selective gas uptake for the natural gas purification and industrial separation. A suitable force field is selected in order to predict the exact experimental outcomes. It is found that the single –Cl functionalization in the organic linker of ZIF-69 has greater inductive effect, which dictates the interactions of gas molecules at the confinement. The predicted interactions directly correlate with the heat of adsorption and selectivity. This study infers that ZIF-68 will work as a gas storage material whereas ZIF-69 works as an excellent candidate for selective capture of methane from natural gas and industrial pollutants.	3	https://www.sciencedirect.com/science/article/abs/pii/S0167577X21012726	2021

Dr. Prakash Muthuramalingam	RSC Advances	Isostructural cocrystals of metaxalone with improved dissolution characteristics	Muscle relaxant and pain reliever metaxalone (MET) is a biopharmaceutical classification systems (BCS) class II drug with poor aqueous solubility and high permeability. The presence of an aromatic skeleton and cyclic carboxamate moiety are the probable reasons for the decreased aqueous solubility, which impacts on its low bioavailability. A high dose (800 mg) of the drug often creates adverse side effects on the central nervous system that needs urgent remedy. Cocrystallization of MET with nicotinamide (NAM), salicylamide (SAM), and 4-hydroxybenzoic acid (HBA) resulted in multicomponent solids that were characterized by PXRD, DSC and single crystal X-ray diffraction. Cocrystals with SAM and NAM form 2D isostructural cocrystals, whereas with HBA the result is a differently packed cocrystal hydrate (or anisole hemisolvate) depending upon the crystallization medium. Similar to the reported MET cocrystals, these cocrystals also confirm the preference for an imide imide homosynthon in the drug. The dominance of the drug–drug homodimer over drug-coformer heterodimers was demonstrated based on binding energy calculations. Further, powder dissolution experiments in pH 6.8 phosphate buffer indicate that the cocrystals improved the apparent solubility compared to the native drug by 3–9 fold. The absence of stronger heterosynthons between MET and the coformers, their lower melting points and the high solubility of the coformers are the probable reasons for the enhanced solubility of the bioactive component. The MET–NAM cocrystal exhibited the highest solubility/dissolution rate among the three binary solid forms, which may offer improved bioavailability and a lower dose with minimal side effects.	3.9	https://pubs.rsc.org/en/content/articlelanding/2021/ra/d1ra05959a	2021
Dr. Prakash Muthuramalingam	Energy & Fuels	Correlation Study on Biopolymer-Blended Cobalt and Iodine Gel Electrolytes to Enhance the Efficiency of Natural Dye-Based DSSCs	In this study, we prepared a new natural sensitizer from blood berry extract (BB dye) and coupled it with a series of biopolymer gel electrolytes consisting of Co2+/3+ or I–/I3–, such as GE 1, GE 2, GE 3, GE 4, GE 5, and GE 6. An as-prepared natural dye was characterized via UV–visible spectroscopy to confirm the behavior of the dye, which showed an absorption range at 484 nm. The interaction between the TiO2 surface and the BB dye was analyzed by density functional theory (DFT) studies. All six biogel electrolytes were characterized using Fourier transform infrared (FTIR), UV, X-ray diffraction (XRD), differential scanning calorimetry (DSC), scanning electron microscopy (SEM), and cyclic voltammetry (CV) techniques to validate the integration of redox mediators into polymer hosts. The bioelectrolytes GE 1, GE 2, GE 4, and GE 5 contain a single polymer matrix (xanthan gum or gelatin) and showed a very low photo-conversion efficiency. At the same time, GE 3 and GE 6 contain a blended polymer matrix (xanthan gum and gelatin) and achieved a higher power conversion efficiency (PCE) of 0.86 and 2.06%, respectively, under 1 sun illumination. The redox mediator Co2+/3+ or I–/I3– incorporated into both single and blended polymer matrixes played a vital role in regenerating the BB dye. In this case, the bioblended polymer gel electrolyte (GE 6) consisting of a Co2+/3+ redox pair attained a high conductivity of 5.97 × 10–5 S/cm–1 and a chemical capacitance of 15.02 ×10–6 F compared to the I–/I3–-incorporated electrolyte. The PCE reports were sustained by the electrochemical impedance spectrum results such as a larger charge at the Pt/electrolyte interface, a lower charge transfer resistance at the TiO2/dye/electrolyte interface, and a higher chemical capacitance. The introduction of a biopolymer cobalt redox-based gel electrolyte with the natural BB dye improves the electron lifetime and readily reduces the recombination reaction. The integration of a natural dye with a blended biopolymer gel electrolyte can pave the way to generate new eco-friendly dye-sensitized solar cells (DSSCs) with high stability.	5.3	https://pubs.acs.org/doi/abs/10.1021/acs.energyfuels.1c02264	2021

Dr. Prakash Muthuramalingam	Physical Chemistry Chemical Physics	The molecular mechanism behind the stabilization of insulin by choline and geranate (CAGE) ionic liquids – computational insights into oral insulin drug formulation	Insulin is a principal hormone that is involved in the regulation of glucose levels in the blood. Oral insulin formulation is a recent development in drug delivery systems. Biocompatible choline-based ionic liquids (ILs) show promising antibacterial activity and are useful for oral and transdermal drug delivery applications. Choline and geranate (CAGE) ILs enhance the stability and oral efficacy of insulin delivery. The molecular mechanism behind insulin formulation in the oral form is at issue. In the present work, the molecular-level understanding of CAGE ILs in insulin is scrutinized by employing atomistic molecular dynamics (MD) simulations. To identify the stability of insulin in an IL medium, we have studied a series of concentration (mole fraction 0.05–1.00) of CAGE ILs with an insulin dimer. It can be well evidenced from the experimental reports that in an aqueous medium, there is a refashioning of CAGE nanostructures at 0.50 mole fraction. It is found from our calculations that the first solvation shell of insulin is readily occupied by choline and geranate ions in the presence of water. Moreover, the geranate ions strongly interacted with the water molecules and thereby, eliminating the intermolecular hydrogen bonding (H-bonding) interactions towards the insulin at 0.30–0.50 mole fraction of CAGE ILs. The most desirable 0.30–0.50 mole fraction of CAGE invigorates water-mediated H-bonding interactions with geranate ions, which also enhances the electrostatic behavior around the vicinity of the insulin dimer. These important findings can help in the development of oral insulin drug delivery and related applications.	3.3	https://pubs.rsc.org/en/content/articlelanding/2021/cp/d1cp03349b	2021
Dr. Prakash Muthuramalingam	Chemosphere	Carbon dioxide adsorption and activation on ionic liquid decorated Au(111) surface: A DFT study	We use first principles approaches to study the adsorption and catalytic activation mechanism of CO2 on ionic liquids (ILs, [CnMIm]$^{+}$[Cl]$^{-}$ (n = 0–6)) attached to a Au(111) surface. The adsorption of CO2 at this liquid-solid model interface occurs via either (i) parallel π-stacking mode or (ii) CO2 oxygen lone pair (lp)···π interaction. These CO2 physisorption modes, which depend on the CO2 landing angle at this interface, are identified as an efficient way to activate CO2 and its further conversion into value-added products. For illustration, we discuss the conversion of CO2 into formic acid where the (111) decorated interface allows reduction of the activation energy for the CO2 + H2 → HCOOH reaction. In sum, our electrode/electrolyte based interface model provides valuable information to design novel heterogeneous catalysts for CO2 conversion. Indeed, our work establishes that a suitable interface material is enough to activate CO2.	8.8	https://www.sciencedirect.com/science/article/abs/pii/S0045653521020841	2022
Dr. Prakash Muthuramalingam	Journal of Colloid and Interface Science	Identification of a Grotthuss proton hopping mechanism at protonated polyhedral oligomeric silsesquioxane (POSS) – water interface	The attachment and dissociation of a proton from a water molecule and the proton transfers at solid–liquid interfaces play vital roles in numerous biological, chemical processes and for the development of sustainable functional materials for energy harvesting and conversion applications. Using first-principles computational methodologies, we investigated the protonated forms of polyhedral oligomeric silsesquioxane (POSS-H+) interacting with water clusters (Wn, where n = 1–6) as a model to quantify the proton conducting and localization ability at solid–liquid interfaces. Successive addition of explicit water molecules to POSS-H+ shows that the assistance of at least three water molecules is required to dissociate the proton from POSS with the formation of an Eigen cation (H9O4+), whereas the presence of a fourth water molecule highly favors the formation of a Zundel ion (H5O2+). Reaction pathway and energy barrier analysis reveal that the formation of the Eigen cation requires significantly higher energy than the Zundel features. This confirms that the Zundel ion is destabilized and promptly converts in to Eigen ion at this interface. Moreover, we identified a Grotthuss-type mechanism for the proton transfer through a water chain close to the interface, where symmetrical and unsymmetrical arrangements of water molecules around H+ of protonated POSS-H+ are involved in the conduction of proton through water wires where successive Eigen-to-Zundel and Zundel-to-Eigen transformations are observed in quick succession.	9.9	https://www.sciencedirect.com/science/article/abs/pii/S0021979721011759	2022

Dr. Prakash Muthuramalingam	Inorganica Chimica Acta	Synthesis and antiproliferative activity of novel organometallic cobalt(III) complex encapsulated in polydiacetylene-phospholipid nanoformulation	Organometallic complexes are considered as promising anticancer agents with the aim to overcome the limitations of platinum drugs but until very recently the development of organometallic cobalt-based anticancer active compounds has remained scarce. Two novel half-sandwich Cobalt(III)-pentamethylcyclopentadienyl complexes containing Schiff base ligands of the general formula [Cp*Co(NN)CH3CN](ClO4)2(Cp*Co(L1) and Cp*Co(L2)), where Cp* is pentamethylcyclopentadiene and NN is bis(anthracen-9-ylmethylene)benzene-1,2-diamine (L1) or bis(4-isopropylbenzylidene)benzene-1,2-diamine (L2), have been synthesized and characterized by elemental analysis, spectroscopic techniques, DFT method and cyclic voltammogram analysis. The facile reduction behaviour of complexes illustrates the observed potency of their oxidative DNA cleavage. Cp*Co(L1) complex displays oxidative DNA cleavage in presence of ascorbic acid more prominent than Cp*Co(L2) by generating radical dotOH radicals. Cp*Co(L1) complex shows remarkable cytotoxicity (IC50: 0.5 µM) towards A549 lung and HeLaS3 cervical cancer cells but moderate to normal human lung fibroblast cells (IC50: 6.02 µM). Also, the cytotoxic potency of Cp*Co(L1) is significantly higher than its analogue complex as well as cis-platin due to its redox behaviour and enhanced hydrophobicity of the ligand moieties. The AO/EB staining assay reveals that the complexes are able to induce late apoptotic mode of cell death in lung and cervical cancer cells. In order to improve the biocompatibility and anticancer activity of Cp*Co(L1) complex, it is encapsulated into polymer-supported liposomes and the size and morphology of nanoformulation is characterized by suitable techniques. The toxic effect of the complex after being encapsulated into liposome is reduced towards normal cells. However, the nanoformulation is less active in lung and cervical cancer cells compared to non-encapsulated complex.	2.8	https://www.sciencedirect.com/science/article/abs/pii/S0020169321004576	2022
Dr. Prakash Muthuramalingam	Computational and Theoretical Chemistry	Simultaneous interaction of graphene nanoflakes with cations and anions: A cooperativity study	We have investigated the structure and the stability of ternary complexes, made up of an extended aromatic π-surface that simultaneously interacts with cation and anion on the opposite faces of the aromatic π-cloud. To understand the influence of the role of aromatic surfaces in the ternary complexes, we have considered various linear and circular polycyclic aromatic hydrocarbons (PAHs) as model systems for the extended π-electron surface. The interplay between the structure, stability, and cooperativity is studied using density functional theory (DFT) methods. Furthermore, the nature of the interaction, energetics, and origin of cooperative effects in the ternary complexes are characterized by using atoms in molecules (AIM), nucleus independent chemical shift (NICS), and energy decomposition analyses (EDA). Results obtained from these calculations unravel the cooperative effects present in the ternary complexes and the interplay between cation···π and anion···π interactions when they coexist in the same system.	2.8	https://www.sciencedirect.com/science/article/abs/pii/S2210271X22000147	2022

Dr. Prakash Muthuramalingam	RSC Advances	Antiviral activities of natural compounds and ionic liquids to inhibit the Mpro of SARS-CoV-2: a computational approach	The recalcitrant spread of the COVID-19 pandemic produced by the novel coronavirus SARS-CoV-2 is one of the most destructive occurrences in history. Despite the availability of several effective vaccinations and their widespread use, this line of immunization often faces questions about its long-term efficacy. Since coronaviruses rapidly change, and multiple SARS-CoV-2 variants have emerged around the world. Therefore, finding a new target-based medication became a priority to prevent and control COVID-19 infections. The main protease (Mpro) is a salient enzyme in coronaviruses that plays a vital role in viral replication, making it a fascinating therapeutic target for SARS-CoV-2. We screened 0.2 million natural products against the Mpro of SARS-CoV-2 using the Universal Natural Product Database (UNPD). As well, we studied the role of ionic liquids (ILs) on the structural stabilization of Mpro. Cholinium-based ILs are biocompatible and used for a variety of biomedical applications. Molecular docking was employed for the initial screening of natural products and ILs against Mpro. To predict the drug-likeness features of lead compounds, we calculated the ADMET properties. We performed MD simulations for the selected complexes based on the docking outcomes. Using MM/PBSA approaches, we conclude that compounds NP-Hit2 (−25.6 kcal mol−1) and NP-Hit3 (−25.3 kcal mol−1) show stronger binding affinity with Mpro. The hotspot residues of Thr25, Leu27, His41, Met49, Cys145, Met165, and Gln189 strongly interacted with the natural compounds. Furthermore, naproxenate, ketoprofenate, and geranate, cholinium-based ILs strongly interact with Mpro and these ILs have antimicrobial properties. Our findings will aid in the development of effective Mpro inhibitors.	3.9	https://pubs.rsc.org/en/content/articlehtml/2022/ra/d1ra08604a	2022
Dr. Prakash Muthuramalingam	ACS Applied Energy Materials	Boron-Induced Cationic Vacancy on Copper Cobalt Oxide toward Formate Selectivity: New Insights into Methanol Oxidation Reaction	In noble metal-based fuel cells, adsorbed carbon monoxide plays a vital role in hindering their efficiency. To alleviate this problem, constructing non-noble metals, particularly selective toward formate formation, will be an ideal solution. Further, to improve the electrochemical properties, we deliberately introduced point defects, namely, cationic vacancies. Herein, we have chosen boron as a dopant that introduces the cationic vacancy in copper cobalt oxide (B/CuCo2O4) and improves the methanol absorption capability. Our synthesized B/CuCo2O4 electrocatalyst showed 91 mA cm−2 (4-fold) higher current density than the pristine electrocatalyst. Most importantly, unlike noble metals, our synthesized electrocatalyst was selective toward formate formation and obtained a faradic efficiency of 43% as demonstrated by NMR, and the reaction pathway was predicted by density calculation theory.	6.4	https://pubs.acs.org/doi/abs/10.1021/acsaem.1c03643	2022
Dr. Prakash Muthuramalingam	ECS Transactions	Role of Functional Groups in ILs Decorated Au (111) Surface for CO2 Capture and Activation: A First Principle Approach	A heterogeneous catalytic environment plays a major role to decide the catalytic activation and conversion of the CO2 molecule at the interface. For this, we have chosen functionalized 1-ethyl-3-methylimidazolium cation (i.e. [EMIm-Z]+[X]-, where Z = NH2 and CF3) with two different anions (i.e. [X]- = [DCA]- and [SCN]-). Our results reveal that the electron donating groups at the interface can effectively activates and converts CO2 to radical anion. But the electron-withdrawing (i.e. –CF3) substituent lowers the binding strength of CO2. Besides, the adsorption and activation mechanism of CO2 at the interface is directly influenced by the involvement of the -NH2 functional groups in the ([EMIm]+) cation. It is identified that the different types of intermolecular interactions between the CO2 and interface. Such as (i) O=C=O····H(-NH2), (ii) O=C=O····H (-CH3)), (iii) O=C=O····F(-CF3). Our work provides a clear picture about the role of the functional group at the interfacial medium for activation of CO2.	0.63	https://iopscience.iop.org/article/10.1149/10701.11383ecst/meta	2022

Dr. Prakash Muthuramalingam	ECS Transactions	The Inhibition Activity of Natural Products Against Host and Viral Proteins Of SARS-Cov-2: Computational Perspective	The Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) has disseminated worldwide, decimating millions of people. The number of illnesses and deaths will rise exponentially since there are no viable medications. Especially, with the complex mutations spreading worldwide, the design and development of effective drugs are much needed. Herein, to understand the molecular interactions and mode of binding, 100 natural compounds were tested against Main protease (Mpro), Receptor Binding Domain (RBD) of SARS-CoV-2, and human Angiotensin-converting enzyme 2 (hACE2) using molecular docking. Molecular dynamics simulations were conducted for a period of 100 ns for the best 3 compounds with each target to validate the stability of the complexes. RMSD, RMSF, and Rg analyses were performed to determine the structure and stability of protein-ligand complexes. Further, binding free energy calculations were performed using MM/PBSA approach to identify the effective antiviral agents. Our results will render the potent inhibitors of SARS-Cov-2.	0.63	https://iopscience.iop.org/article/10.1149/10701.11397ecst/meta	2022
Dr. Prakash Muthuramalingam	ECS Transactions	Screening of Suitable Size/Pore Dependent IL/UiO-66 Composite for Selective Gas Separation Application	The separation of toxic gases is the imperative environmental demand for which the isostructural UiO-66 metal-organic framework (MOF) has captivated, due to its exceptional thermal and chemical stability. There are two types of pores, the larger octahedral (Oh) pore (i.e., ~16 Å) and the smaller tetrahedral (Td) pore (i.e., ~10 Å), and they both perform differently in adsorbing the gas molecules. To enhance the gas separation application, green solvent ionic liquids (IL) are impregnated. The enormous application lies in its cation-anion tunability. Our interest is to find the most suitable pore for IL occupancy in UiO-66 for effectual CO2 separation. To comprehend the IL interaction inside the pores, [BMIM]+[X]- and [EMIM]+[X]- (Where X = Cl, BF4, PF6, HCOO, and CF3COO) in Oh and Td pores of UiO-66 are studied using the first principle approach. We observe the selectivity and adsorption of composites for selecting the suitable composite for gas separation application. Among the high BE composites, we found [BMIM][PF6]Oh@UiO-66 shows promising selectivity and adsorption.	0.63	https://iopscience.iop.org/article/10.1149/10701.13625ecst/meta	2022
Dr. Prakash Muthuramalingam	Frontiers in Chemistry	Design of Ascorbic Acid Eutectic Mixtures With Sugars to Inhibit Oxidative Degradation	L-Ascorbic acid (ASC), commonly known as vitamin C, acts as an anti-oxidant in the biological system. It is extensively used as an excipient in pharmaceutical industry, food supplements in fruit juices, and food materials due to its free radicals scavenging activity. Main drawback of ASC is its poor aqueous stability owing to the presence of lactone moiety that is easily oxidized to dehydroascorbic acid and further degraded. To improve aqueous stability and inhibit oxidative degradation, ASC was co-crystallized to constitute binary eutectic compositions with mono and di-saccharides such as glucose, sucrose, lactose, and mannitol. The eutectics were confirmed by their (single) lower melting endotherm compared to ASC and sugars, although Powder X-ray diffraction (PXRD) and Fourier transform Infrared spectroscopy (FT-IR) data confirmed the characteristics of their physical mixture. Scanning electron microscope (SEM) images of the binary eutectics confirmed their irregular morphology. The ASC eutectics exhibited improved shelf-life by 2–5-fold in weakly acidic (pH 5) and neutral (pH 7) aqueous buffer medium, whereas the eutectic with glucose enhanced shelf-life only by 1.1–1.2-fold in acidic medium (pH 3.3 and 4). Notably, stabilizing effect of the sugar eutectics decreased with increasing acidity of the medium. In addition, higher binding energy of the disaccharide eutectics partially supports the aqueous stability order of ASC in the neutral pH medium due to more number of non-bonded interactions than that of monosaccharides.	5.5	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC9125031/	2022

Dr. Prakash Muthuramalingam	Journal of Materials Science: Materials in Electronics	Enhancing the thermoelectric performance by defect structures induced in p-type polypyrrole-polyaniline nanocomposite for room-temperature thermoelectric applications	Organic thermoelectric materials mainly conducting polymers are green materials that can convert heat energy into electrical energy and vice versa at room temperature. In the present work, we investigated the thermoelectric properties of polymer nanocomposite of polypyrrole (PPy) and polyaniline (PANI) (PPy/PANI) by varying the pyrrole: aniline monomer ratios (60:40, 50:50, and 40:60). The PPy/PANI composite is prepared by in-situ chemical polymerization of PPy on PANI dispersion. It has been observed that the combination of two conducting polymers has enhanced the electrical and thermal properties in the PPy/PANI composite due to the strong π–π stacking and H-bonding interaction between the conjugated structure of PPy and conjugated structure of PANI. The maximum electrical conductivity of 14.7 S m−1 was obtained for composite with high pyrrole content, whereas the maximum Seebeck coefficient of 29.5 µV K−1 was obtained for composite with high aniline content at 366 K. Consequently, the PPy/PANI composite with pyrrole to aniline monomer ratio of 60:40 exhibits the optimal electrical conductivity, Seebeck coefficient, and high power factor. As a result, the maximum power factor of 2.24 nWm−1 K−2 was obtained for the PPy/PANI composite at 60:40 pyrrole to aniline monomer ratio, which is 29 times and 65.8 times higher than PPy (0.077 nWm−1 K−2) and PANI (0.034 nWm−1 K−2), respectively.	2.8	https://link.springer.com/article/10.1007/s10854-022-08112-0	2022
Dr. Prakash Muthuramalingam	Journal of Electrochemical Society	Role of Functional Groups in an Ionic Liquid Decorated Au(111) Surface for CO2 Capture and Activation: A First Principle Approach	A heterogeneous catalytic environment plays a major role to decide the catalytic activation and conversion of the CO2 molecule at the interface. For this, we have chosen functionalized 1-ethyl-3-methylimidazolium cation (i.e. [EMIm-Z]+[X]−; Where, Z = NH2 and CF3) with two different anions (i.e. [X]− = [DCA]− and [SCN]−). Our results reveal that the electron-donating groups at the interface can effectively activate and converts CO2 to radical anion. But the electron-withdrawing (i.e. –CF3) substituent lowers the binding strength of CO2. Besides, the adsorption and activation mechanism of CO2 at the interface is directly influenced by the involvement of the –NH2 functional groups in the ([EMIm]+) cation. It is identified that the different types of intermolecular interactions between the CO2 and interface. Such as, (i) O = C = O····H(–NH2) (ii) O=C=O····H (–CH3)) (iii) O=C=O····F(–CF3). Our work provides a clear picture of the role of the functional group in the interfacial medium for the activation of CO2.	3.9	https://iopscience.iop.org/article/10.1149/1945-7111/ac71d6	2022
Dr. Prakash Muthuramalingam	Molecules	Counteractive Effects of Choline Geranate (CAGE) ILs and Ethanol on Insulin's Stability-A Leap Forward towards Oral Insulin Formulation	Choline geranate (CAGE) ionic liquids (ILs) stabilize insulin, thereby aiding its oral delivery, whereas ethanol (EtOH) affects its stability by disrupting the hydrophobic interactions. In this study, cognizance of the stabilization mechanism of insulin dimer in the presence of both CAGE ILs and EtOH mixtures is achieved through biased and unbiased molecular dynamics (MD) simulations. Here, two order parameters are employed to study the insulin dimer dissociation using well-tempered metadynamics (WT-MetaD). The stability of insulin is found to be strongly maintained until a 0.20 mole fraction of EtOH. Besides, higher concentrations of EtOH marginally affect the insulin stability. Moreover, geranate anions form a higher number of H-bonding interactions with water molecules, which aids insulin stabilization. Conversely, the addition of EtOH minimizes the water-mediated H-bonding interactions of geranate. Additionally, geranate traps the EtOH molecules, thereby preventing the interactions between insulin and EtOH. Furthermore, the free energy landscape (FEL) reveals the absence of dimer dissociation along with noticeable deviations in the distances R and the number of contacts Q. The dimerization free energy of insulin was calculated to be -16.1 kcal/mol at a 0.20 mole fraction of EtOH. Moreover, increments in mole fractions of EtOH effectuate a decrease in the insulin stability. Thus, the present study represents CAGE ILs as efficient insulin dimer stabilizes at low concentrations of EtOH.	4.6	https://www.mdpi.com/journal/molecules	2022

Dr. Prakash Muthuramalingam	Physical Chemistry Chemical Physics	Fragmentation dynamics of CH3Clq+ (q = 2,3): theory and experiment	A combined theoretical and experimental study of the dissociation of the di- and trication of the CH3Cl molecule has been performed. Experimentally, these multi-charged ions were produced after interactions of a CH3Cl effusive jet with a mono-energetic beam of H+ or Ar9+ projectile ions. Theoretically, we mapped the multi-dimensional potential energy surfaces of CH3Cl2+, H2CClH2+ and CH3Cl3+ species in their electronic ground and electronically excited states using post-Hartree–Fock configuration interaction methods. In addition to the obvious bond-breaking ionic fragments (i.e. H+ + CH2Cl+, H+ + CH2Cl2+ and CH3+ + Cl+), the formation of H2+ (+CHCl+ or CHCl2+), H3+ (+CCl+) and HCl+ (+CH2+) was observed upon bond rearrangement after ion impact of CH3Cl. The interaction strength of the incident projectiles is found to affect the relative yields on the observed dissociation channels, however, it has no effect on the kinetic energy releases of the fragmentation pathways. For the observed dissociation channels, plausible formation mechanisms were proposed. These reaction pathways take place on the ground and/or electronic excited potential energy surfaces of the doubly and triply charged CH3Cl ions, where spin–orbit and vibronic couplings are in action. Moreover, this work suggests that the mechanisms undertaken may depend on the multiply charged ion preparation by valence or inner-shell single photon photoionization, fast ion beam impact or ultrafast intense laser ionization.	3.3	https://pubs.rsc.org/en/content/articlehtml/2021/cp/d2cp02194c	2022
Dr. Prakash Muthuramalingam	Optical Materials	Effect of end groups on fluorene based dyes without carboxyl anchors as efficient co-sensitizer for retarding charge recombination in DSSC applications	Herein, simple A- π-D- π-A type fluorene-based metal-free organic dyes denoted as DICTF and DRCTF, carrying different terminal units without carboxylic acid were synthesize and utilizes as effective co-sensitizer. By tuning the electron-accepting cyanated terminal units in the dyes, their photo physical, electrochemical and photovoltaic properties were investigated. After stepwise co-sensitization of TiO2 photoanode with DRCTF/N-719 shows a PCE (Power Conversion Efficiency) of 8.22% which is higher than that of bare N-719 alone (4.23%) or higher than for the device co-sensitized with DICTF/N-719 (6.54%). The PCE of the N-719 dye is improved by co-sensitization with the dyes DICTF and DRCTF, clearly reflects in both short circuit current and open-circuit voltage results. EIS (Electrochemical Impedance Spectroscopy) analysis reveals the slow recombination kinetics and extended electron life time of the co-sensitized devices compared with N-719 dye-sensitized alone. Hence, a new stepwise co-sensitization strategy has been implemented in which, the main sensitizer has carboxyl anchors and the co-sensitizer does not have an anchoring group. This helps to boost the performances in the DSSC (Dye sensitized solar cells) by receiving panchromatic absorption and reducing the dye aggregation caused wherein N-719 dye is co-sensitized with DICTF or DRCTF.	3.9	https://www.sciencedirect.com/science/article/abs/pii/S092534672201196X	2022

Dr. Prakash Muthuramalingam	Journal of Biomolecular Structure and Dynamics	Discovery of novel HDAC8 inhibitors from natural compounds by in silico high throughput screening	A class I histone deacetylase HDAC8 is associated with several diseases, including cancer, intellectual impairment and parasite infection. Most of the HDAC inhibitors that have so far been found to inhibit HDAC8 limit their efficacy in the clinic by producing toxicities. It is therefore very desirable to develop specific HDAC8 inhibitors. The emergence of HDAC inhibitors derived from natural sources has become quite popular. In recent decades, it has been shown that naturally occurring HDAC inhibitors have strong anticancer properties. A total of 0.2 million natural compounds were screened against HDAC8 from the Universal Natural Product Database (UNPD). Molecular docking was performed for these natural compounds and the top six hits were obtained. In addition, molecular dynamics (MD) simulations were used to evaluate the structural stability and binding affinity of the inhibitors, which showed that the protein-ligand complexes remained stable throughout the 100 ns simulation. MM-PBSA method demonstrated that the selected compounds have high affinity towards HDAC8. We infer from our findings that Hit-1 (-29.35 kcal mol-1), Hit-2 (-29.15 kcal mol-1) and Hit-6 (-30.28 kcal mol-1) have better binding affinity and adhesion to ADMET (absorption, distribution, metabolism, excretion and toxicity) characteristics against HDAC8. To compare our discussions and result in an effective way. We performed molecular docking, MD and MM-PBSA analysis for the FDA-approved drug romidepsin. The above results show that our hits show better binding affinity than the compound romidepsin (-12.03 ± 4.66 kcal mol-1). The important hotspot residues Asp29, Ile34, Trp141, Phe152, Asp267, Met274 and Tyr306 have significantly contributed to the protein-ligand interaction. These findings suggest that in vitro testing and additional optimization may lead to the development of HDAC8 inhibitors.Communicated by Ramaswamy H. Sarma.	4.4	https://pubmed.ncbi.nlm.nih.gov/36369945/	2023
Dr. Prakash Muthuramalingam	Journal of Molecular Structure	Cyclo[18]carbon-A new class of electron acceptor for organic solar cells applications	The all-carboatomic ring, cyclo[18]carbon (C18), has the potential to act as an electron acceptor due to promising electronic and optical properties. In this study, we first illustrated the geometrical, electronic, and excited-state properties of C18 using various hybrid and long-range corrected density functional theory (DFT) methods. Further, we studied the nature of intermolecular interactions between dimers of C18 to gain insights into packing configurations of cyclo[18] in dimer and trimer configurations. Also, using the state-of-the-art DFT methods, we have reported the thorough characterization of the lowest excited-state (i.e. charge-transfer state) in various donor-acceptor model complexes based on pentacene and C18. We established an interplay between the molecular packing of C18 and pentacene molecules on the energy of charge transfer state. All these results could help in the designing of more efficient organic solar cells.	3.8	https://www.sciencedirect.com/science/article/abs/pii/S0022286022016763	2023

Dr. Prakash Muthuramalingam	Journal of Colloid and Interface Science	Investigation of non-covalent interactions in Polypyrrole/Polyaniline/Carbon black ternary complex for enhanced thermoelectric properties via interfacial carrier scattering and π-π stacking	The thermoelectric (TE) performance of conducting polymers can be improved by the incorporation of carbon nanomaterials. In this work, the impact of carbon black (CB) on polypyrrole (PPy) and polypyrrole/polyaniline (PPy/PANI) binary composite have been investigated. Herein, PPy/PANI binary composite was initially prepared through chemical oxidative polymerization and then solution mixed with CB to form PPy/PANI/CB ternary nanocomposite. The structural and morphological analyses confirmed the formation of composites, and the strong interaction present between polymer matrix and CB. This was further confirmed by theoretical study, which showed strong noncovalent interaction and high complex stability between the materials. The thermoelectric results showed that both the electrical conductivity (σ) and Seebeck coefficient (S) has been increased with the increase in CB content (from 10 wt% to 30 wt%) and temperature (303 K to 373 K), while the thermal conductivity (κ) increase was low. The ternary nanocomposite involving 30 wt% of CB was found to be the most promising material which showed an enhanced power factor (PF) of 0.0251 µW/mK2 and high figure of merit (ZT) of 4.37x10-5 at 370 K. The enhancement in ZT for PPy/PANI/CB ternary composite is 2 times, 316 times, 17.3 times, 3.97 times, 11.7 times, and 6.8 times greater than other samples. The enhancement in power factor and ZT was due to energy filtering effect and strong non-covalent interactions between the homopolymers and CB.	9.9	https://www.sciencedirect.com/science/article/abs/pii/S0021979722016319	2023
Dr. Prakash Muthuramalingam	Molecular Simulation	In silico screening of potential antiviral inhibitors against SARS-CoV-2 main protease	Respiratory illness due to SARS-CoV-2 emerged in 2019 and has a significant morbidity and mortality rate. The main protease (Mpro) is mainly responsible for viral replications, which acts as a good drug target to inhibit SARS-CoV-2-related diseases. Chemical compounds obtained from various herbal plants are showing potent antiviral activity against numerous viral diseases. Initial screening was performed with the phytochemicals against Mpro using molecular docking. This result shows that there is a strong interaction exhibited between active sites (His-41 and Cys-145) of Mpro with chemical compounds. In addition, ADME prediction and Lipinski’s rule of five (RO5) calculations demonstrated that the selected compounds have potential drug-like properties. Further, molecular dynamics (MD) simulations were performed to understand the stability and structural changes of protein–ligand complexes for the top five compounds. MM/PBSA studies strongly suggested that compounds, β-spinasterol, and asarinin form stable complexes with Mpro. The most significant hot spot residues such as Thr-25, Met-49, Cys-145, Met-165, and Gln-189 have strongly interacted with the selected chemical compounds. Our calculations suggest that asarinin is the best inhibitor to the Mpro, which supports these candidates and could be potent antiviral agent against SARS-CoV-2.	2.1	https://www.tandfonline.com/doi/full/10.1080/08927022.2022.2136392	2023

Dr. Prakash Muthuramalingam	Chemical Biology & Drug Design	Compounds from diverse natural origin against triple-negative breast cancer: A comprehensive review	Triple-negative breast cancer (TNBC) is caused due to the lack of estrogen receptors (ER), progesterone receptors (PR), and human epidermal growth factor 2 (HER2) expression. Triple-negative breast cancer is the most aggressive heterogeneous disease that is capable of producing different clones and mutations. Tumorigenesis in TNBC is caused due to the mutation or overexpression of tumor suppressor genes. It is also associated with mutations in the BRCA gene which is linked to hereditary breast cancer. In addition, PARP proteins and checkpoint proteins also play a crucial function in causing TNBC. Many cell signaling pathways are dysregulated in TNBC. Even though chemotherapy and immunotherapy are good options for TNBC treatment, the response rates are still low in general. Many phytochemicals that are derived from natural compounds have shown very good inhibitions for TNBC. Natural compounds have the great advantage of being less toxic, having lesser side effects, and being easily available. The secondary metabolites such as alkaloids, terpenoids, steroids, and flavonoids in natural products make them promising inhibitors of TNBC. Their compositions also offer vital insights into inhibitory action, which could lead to new cancer-fighting strategies. This review can help in understanding how naturally occurring substances and medicinal herbs decrease specific tumors and pave the way for the development of novel and extremely efficient antitumor therapies.	3	https://onlinelibrary.wiley.com/doi/abs/10.1111/cbdd.14172	2023
Dr. Prakash Muthuramalingam	Materials Today Sustainability	Theoretical studies on the role of water in ionic liquids at ZIF (IL@ZIF) complex and its effect on selective CO2 separation	One of the major problems we have always faced and still facing is the vast amount of toxic gases expelled into the atmosphere mainly during the manufacture of many of the day-to-day commodities we all use. The selective adsorption and storage of gases from various industrially important gaseous mixtures are studied in order to find a suitable method as a sustainable solution for this concern. This study is conducted in order to get a perspective on the gas separation and storage capabilities of large framework molecules like zeolitic imidazolate frameworks (ZIFs) by incooperation of ionic liquids (ILs). Here, the gas adsorption efficiency of IL@ZIF-8 composite materials is studied in the presence of a single water molecule. We have selected 1-butyl-3-methylimidazolium [BMIM]+ cation along with five different anions as the ILs. We used both hydrophilic and hydrophobic ILs in this study. The IL@ZIFs complexes are prepared by adding ILs in two different approaches to the ZIF pore. A single water molecule is added into the previously optimized geometries of IL@ZIF in the first method (Approach-I), while we added water and an IL to the ZIF simultaneously in the second method (Approach-II). The selection of the different approaches for water addition helps to gather information about the interaction pattern of water with the IL and ZIF and also of these molecules with one another in the presence of water. We used these complexes to study their adsorption capabilities towards CO2 and also their selectivity nature towards CO2 in a binary mixture of CO2 and N2. Computational approaches such as density functional theory (DFT) and grand canonical Monte Carlo (GCMC) are used in this study.	7.8	https://www.sciencedirect.com/science/article/abs/pii/S2589234723000623	2023

Dr. Prakash Muthuramalingam	Journal of Biomolecular Structure and Dynamics	Identification of indole-based natural compounds as inhibitors of PARP-1 against triple-negative breast cancer: A computational study	Triple-negative breast cancer (TNBC) is the most aggressive kind of breast cancer known to mankind. It is a heterogeneous disease that is formed due to the missing estrogen, progesterone and human epidermal growth factor 2 receptors. Poly(ADP-ribose) polymerase-1 (PARP-1) protein helps in the development of TNBC by repairing the cancer cells, which proliferate and spread metastatically. To determine the potential PARP-1 inhibitors (PARPi), 0.2 million natural products from Universal Natural Product Database were screened using molecular docking and six hit compounds were selected based on their binding affinity towards PARP-1. The bio-availability and drug-like properties of these natural products were evaluated using ADMET analysis. Molecular dynamics simulations were conducted for these complexes for 200 ns to examine their structural stability and dynamic behaviour and further compared with the complex of talazoparib (TALA), an FDA-approved PARPi. Using MM/PBSA calculations, we conclude that the complexes HIT-3 and HIT-5 (−25.64 and −23.14 kcal/mol, respectively) show stronger binding energies with PARP-1 than TALA with PARP-1 (−10.74 kcal/mol). Strong interactions were observed between the compounds and hotspot residues, Asp770, Ala880, Tyr889, Tyr896, Ala898, Asp899 and Tyr907, of PARP-1 due to the existence of various types of non-covalent interactions between the compounds and PARP-1. This research offers critical information about PARPi, which could potentially be incorporated into the treatment of TNBC. Moreover, these findings were validated by comparing them with an FDA-approved PARPi.	4.4	https://www.tandfonline.com/doi/abs/10.1080/07391102.2023.2208215	2023
Dr. Prakash Muthuramalingam	Applied Energy Materials	Ti3C2 Quantum Dots Modified 3D/2D TiO2/g-C3N4 S-Scheme Heterostructures for Highly Efficient Photocatalytic Hydrogen Evolution	Photocatalytic hydrogen production is a promising technology to alleviate the problems of energy shortage and environmental pollution faced by human society. In this paper, the S-scheme heterojunction TiO2/g-C3N4 was modified by Ti3C2 quantum dots (QDs) to prepare a three-dimensional/two-dimensional/zero-dimensional (3D/2D/0D) photocatalyst for photocatalytic hydrogen production. The S-scheme heterojunction structure reduces the recombination rate of photogenerated electron–hole pairs and produces more photogenerated electrons. At the same time, Ti3C2 quantum dots as electron acceptors improve the ability to capture transition electrons, obtain more photogenerated carriers involved in surface reactions, and increase the number of active sites. The TiO2/g-C3N4/Ti3C2 QDs composite catalyst shows excellent photocatalytic hydrogen evolution performance under visible light due to its unique structure and optical properties. The photocatalytic hydrogen production rate reached the maxima of 5540.21 µmol·h–1 g–1, which is nearly 2 times higher than the production rates observed for TiO2/g-C3N4. The structure of 3D/2D/0D TiO2/g-C3N4/Ti3C2 QDs was constructed, and the electron transfer path was verified by transient absorption spectroscopy and density functional theory calculation.	6.4	https://pubs.acs.org/doi/10.1021/acsaem.1c03019	2023

Dr. Prakash Muthuramalingam	New Journal of Chemistry	Effect of mixtures of ionic liquids and water on the structure and stability of the insulin dimer: a combined DFT and MD simulation study	Biocompatible cholinium-based ionic liquids (ILs) are used extensively in the pharmaceutical and biomedical industries. To enhance structural stability and solubility of drugs, as well as their controlled delivery, IL-based active pharmaceutical ingredients (API) are used widely. In this study, we selected two different sets of biodegradable ILs which also have a direct influence on the structure and stability of insulin. Moreover, we used DFT-based electronic structure calculations with molecular dynamics (MD) simulations to study the effect of a mixture of two different anions in the IL medium and the role of water molecules on the stability of insulin. Microhydration and molecular-level DFT calculations suggest that ILs based on choline geranate [Cho][Ger] and choline taurine [Cho][Tau] differ in their hydration patterns, and thus the stability of the clusters varies significantly. This finding is important for exploring the role of water molecules within these mixtures (i.e., on the interactions between [Ger] and [Tau]). From our calculations it is found that the [Cho][Ger] IL stabilizes the insulin dimer structure strongly through water-mediated H-bonding interactions, whereas the [Cho][Ger][Tau] ternary complex destabilizes insulin. This indicates that IL mixtures over a wide range of concentrations and water molecules at the interface may influence the structural stability and enable suitable combinations of oral formulations to be predicted for drug-delivery applications. From the MD simulations, we conclude that [Cho][Ger] stabilizes the insulin dimer. Our combined DFT and MD simulations will provide valuable information for experimentalists to design and develop novel oral insulin formulations.	3.3	https://pubs.rsc.org/en/content/articlelanding/2023/nj/d3nj01068f/unauth	2023
Dr. Prakash Muthuramalingam	ChemPhysChem	Formation of Eigen or Zundel Features at Protonated Water Cluster–Aromatic Interfaces	Interfacial interactions of protonated water clusters adsorbed at aromatic surfaces play an important role in biology, and in atmospheric, chemical and materials sciences. Here, we investigate the interaction of protonated water clusters ((H+H2O)n (where n=1–3)) with benzene (Bz), coronene (Cor) and dodecabenzocoronene (Dbc)). To study the structure, stability and spectral features of these complexes, computations are done using DFT-PBE0(+D3) and SAPT0 methods. These interactions are probed by AIM electron density topography and non-covalent interactions index (NCI) analyses. We suggest that the excess proton plays a crucial role in the stability of these model interfaces through strong inductive effects and the formation of Eigen or Zundel features. Also, computations reveal that the extension of the π-aromatic system and the increase of the number of water molecules in the H-bounded water network led to a strengthening of the interactions between the corresponding aromatic compound and protonated water molecules, except when a Zundel ion is formed. The present findings may serve to understand in-depth the role of proton localized at aqueous medium interacting with large aromatic surfaces such as graphene interacting with acidic liquid water. Besides, we give the IR and UV-Vis spectra of these complexes, which may help for their identification in laboratory.	2.9	https://chemistry-europe.onlinelibrary.wiley.com/doi/10.1002/cphc.202300267	2023

Dr. Prakash Muthuramalingam	International Journal of Hydrogen Energy	Holey carbon-nanotube-wrapped MXene for hydrogen evolution reactions and supercapacitor applications	In recent years, interest in noble metal-free catalysts for the hydrogen evolution reaction (HERs) and supercapacitor (SCs) applications has emerging for altering the high-price of the catalyst and prohibiting the dissolution/phase change of the catalysts in long term performances. In this study, we present a novel noble metal-free electrocatalyst composed of holey carbon nanotubes (h-CNTs) and MXene nanocomposites for electrocatalytic HERs and SCs. By wrapping h-CNTs into the surface of the MXene sheet, we address the limitations of pure MXenes and achieve superior electrochemical performance. Specifically, MXenes containing 20 wt% h-CNTs exhibit a low overpotential of 192 mV versus RHE and a small Tafel slope of 48.95 mV dec−1 at 10 mA cm−2 in 0.5 M H2SO4 with excellent cyclic stability. The presence of Cdouble bondO functional groups and the existence of a holey in CNT probably enhanced the electrocatalytic activity. The excellent wrapping of h-CNTs on MXene efficiently exhibited the HER performances because of their individual effect and the arising of synergy, where the excellent interaction attained between the immobilized atom in the h-CNT and MXene. For SCs, MXenes containing 15 wt% h-CNTs display the highest specific capacitance of 404 F g−1 at 4 A/g with excellent cyclic stability, maintaining 80% capacity after 4000 cycles at 10 A/g at ambient temperature in 2 M KOH. Furthermore, the MXene@h-CNT nanocomposite was subjected to density functional theory (DFT) calculation. Our findings demonstrate that the newly developed nanocomposite offers a promising route to boost HER and SCs performance for a wide range of technological applications.	7.2	https://www.sciencedirect.com/science/article/abs/pii/S0360319923030793	2023
Dr. Prakash Muthuramalingam	Inorganic Chemistry Communications	Photocatalytic activities of cadmium(II) acetophenone thiosemicarbazone complex: Experimental and density functional theory based study	The Cd(II) complex of the type CdI2(acetptsczH)2 (where, acetptsczH = acetophenone thiosemicarbazone) has been utilized for photoreduction of Cr(VI) to Cr(III) and photodegradation of methylene blue. The complete reduction of Cr(VI) to Cr(III) and photodegradation of methylene blue was observed in 15 and 120 min respectively. Density functional theory (DFT) produced the highest occupied and lowest unoccupied molecular orbital (HOMO-LUMO) energy gaps, which were important theoretical values to link with the photoreduction and photodegradation activities of the metal complex. The predicted energy gap is 2.60 eV, but DFT calculations show that additional energy is needed to transport an electron from the valance shell. Electronic excitation demonstrates that there is a strong HOMO-1 to LUMO orbital adsorption that correlates with the experimental results. Furthermore, our calculation indicates that the solvent impact (i.e., 2-propanal) has caused a significant change in frequency. Therefore, both experimental and theoretical methods are used to support the photocatalytic activity of the Cd(II) complex. Based on DFT research, the results give an insight into the intended uses of the cadmium complex. The charge transfer and thermal stability of the complex were investigated using cyclic voltammetry (CV) curve.	3.8	https://www.sciencedirect.com/science/article/abs/pii/S1387700323006767	2023

Dr. Prakash Muthuramalingam	ChemistrySelect	The Virtual Screening of Compounds from the ZINC Database against PARP-1 in Triple-Negative Breast Cancer	Triple-negative breast cancer (TNBC) is the most aggressive kind of breast cancer that has disseminated worldwide, decimating millions of people. Especially, since it is capable of forming complex mutations, the design and development of effective drugs are much needed. Clinically, though talazoparib is an FDA-approved drug for PARP against advanced breast cancer, it has several adverse side effects such as anaemia, alopecia, neutropenia and thrombocytopenia. Herein, to understand the molecular interactions and mode of binding, 4.59 million lead-like compounds from the ZINC database were virtually screened against poly(ADP-ribose) polymerase-1 (PARP-1) protein using molecular docking. ADMET analysis were also performed for these compounds. Molecular dynamics (MD) simulations were conducted for a period of 100 ns for the best five compounds to validate the stability of the complexes. Root-mean-square deviation (RMSD), root-mean-square fluctuation (RMSF), and the radius of gyration (Rg) were analyzed and the number of hydrogen bonding interactions was identified to determine the structure and stability of these protein-ligand complexes. Further, binding free energy calculations were performed using the molecular mechanics-Poisson-Boltzmann surface area (MM/PBSA) approach to identify the effective anticancer agents. Z02, Z03, and Z04 have the highest binding affinity of −19.6, −18.1, and −18.1 kcal/mol, respectively, with PARP-1. They also have been found to strongly enhance the stability of the target. All things considered; we determine that compound Z04 is the most promising hit for TNBC.	2.307	https://chemistry-europe.onlinelibrary.wiley.com/doi/abs/10.1002/slct.202304729	2024
Dr. Prakash Muthuramalingam	Journal of Biomolecular Structure and Dynamics	Exploration of novel hydroxamate zinc binding group inhibitors against HDAC-1-3 enzymes by AI-based virtual screening: atomistic insights from steered molecular dynamics	Overexpression of histone deacetylase (HDAC) enzymes is linked to a wide variety of illnesses, including malignancies and neurological disorders, which makes HDAC inhibitors potentially therapeutic. However, most HDAC inhibitors lack subclass or isoform selectivity, which can be dangerous. Featuring both enhanced selectivity and toxicity profiles, slow-binding HDAC inhibitors offer promising treatment options for a variety of disorders. Diseases like cardiac, neurodegenerative disorders and diabetes are mainly associated with the HDAC1, HDAC2 and HDAC3 enzymes. The AI-based virtual screening tool PyRMD is implemented to identify the potential inhibitors from ~2 million compounds. Based on the IC50 values, the top 10 compounds were selected for molecular docking. From the docking and ADMET study, the top-ranked three compounds were selected for molecular dynamics (MD) simulations. Further, to get more insights into the binding/unbinding mechanism of the ligand, we have employed the steered molecular dynamics (SMD) simulations. This study assists in developing Amber force field parameters for the HDAC1, HDAC2 and HDAC3 proteins and sheds light on the discovery of a potent drug. Our study suggests that hydroxamic acid derivative (i.e. referred to as Comp-1, CHEMBL600072) is the potential inhibitor for the series of HDAC-related diseases.	4.4	https://www.tandfonline.com/doi/abs/10.1080/07391102.2024.2325104	2024

Dr. Prakash Muthuramalingam	Journal of Biomolecular Structure and Dynamics	Evaluation of the Efficacy of Marine Natural Products against PARP-1/2 Proteins in High-grade Serous Ovarian Cancer: Insights into MD and SMD Simulations.	High-grade serous ovarian cancer (HGSOC) is the most malignant and ubiquitous phenotype of epithelial ovarian cancer. Originating in the fallopian tubes and rapidly spreading to the ovaries, this highly heterogeneous disease is a result of serous tubal intraepithelial carcinoma. The proteins known as poly(ADP-ribose) polymerase (PARP) aid in the development of HGSOC by repairing the cancer cells that proliferate and spread metastatically. By using molecular docking to screen 1100 marine natural products (MNPs) from different marine environments against PARP-1/2 proteins, prominent PARP inhibitors (PARPi) were identified. Four compounds, alisiaquinone A, alisiaquinone C, ascomindone D and (+)-zampanolide referred to as MNP-1, MNP-2, MNP-3 and MNP-4, respectively, were chosen based on their binding affinity towards PARP-1/2 proteins, and their bioavailability and drug-like qualities were accessed using ADMET analysis. To investigate the structural stability and dynamics of these complexes, molecular dynamics simulations were performed for 200 ns. These results were compared with the complexes of olaparib (OLA), a PARPi that has been approved by the FDA for the treatment of advanced ovarian cancer. We determined that MNP-4 exhibited stronger binding energies with PARP-1/2 proteins than OLA by using MM/PBSA calculations. Hotspot residues from PARP-1 (E883, M890, Y896, D899 and Y907) and PARP-2 (Y449, F450, A451, S457 and Y460) showed strong interactions with the compounds. To comprehend the unbinding mechanism of MNP-4 complexed with PARP-1/2, steered molecular dynamics (SMD) simulations were performed. We concluded from the free energy landscape (FEL) map that PARP-1/2 are well-stabilised when the compound MNP-4 is bound rather than being pulled away from its binding pockets. This finding provides significant evidence regarding PARPi which could potentially be employed in the therapeutic treatment of HGSOC.	4.4	(Revision submitted)	2024
Dr. Prakash Muthuramalingam	Physical Chemistry Chemical Physics	Microhydration of small protonated polyaromatic hydrocarbons: a first principles study	Using first principles methodology, we investigate the microsolvation of protonated benzene (BzH+), protonated coronene (CorH+) and protonated dodecabenzocoronene (DbcH+)). Complexes of these small protonated polyaromatic hydrocarbons (H+PAHs) with mono-, di-, and tri-hydrated water molecules are considered. Their most stable forms are presented, where we discuss their structural, energetic and IR and UV spectral features. In particular, we focus on the analysis of the bounding and various non-bonded interactions between these protonated aromatics and water clusters. The strength of non-bonded interactions is quantified and correlated with their electron density profiles. Further, insights on the interfacial interactions and stability of these complexes were obtained through noncovalent index and symmetry-adapted perturbation theory (SAPT0) analyses. We also discuss the effects of the extension of the ⍰ aromatic cloud on the water solvation of these protonated aromatics. In particular, we extended our predictions for the S0 S1 and S0 T1 wavelength transitions of micro hydrated H+PAHs to deduce those of these species solvated in aqueous solution. These present findings should be useful for understanding, at the microscopic level, of the effects of water interacting with +PAHs, which are relevant for organic chemistry, astrochemistry, atmospheric chemistry, combustion and materials science.	3.3	(Under Revision)	2024
Dr. K. Iyakutti, Dr. V.J. Surya	Materials Science and Engineering: B	18 and 12 – Member carbon rings (cyclo[n]carbons) – A density functional study	Multi-member rings composed of 18 and 12 carbon atoms are designed and stabilised on graphene, the one atom thick carbon substrate, computationally using density functional theory. The resultant structures are intriguing. Bond lengths are found to be equal in both the carbon rings and the atoms are connected through double bonds. The 18-member carbon ring is not circular in shape, whereas the 12-member ring has the circular configuration. The system of 18-member carbon ring on graphene is metallic. Our studies have shown that a weak but definite bonding between the ring structures and the graphene substrate decides the shape of the new carbon allotrope.	4.7	https://www.sciencedirect.com/science/article/abs/pii/S0921510720304025	2021

Dr. K. Iyakutti	Materials Today Communications	Electronic structure, elastic, optical and thermal properties of chalcopyrite CuBY2 (B= In, Ga , In0.5 Ga0.5; Y= S, Se, Te) solar cell compounds	The electronic structure, elastic, optical and thermal properties of chalcopyrite solar cell compounds, CuBY2 (B = In, Ga, In0.5Ga0.5; Y = S, Se, Te) are systematically studied. The crystal structure of ternary semiconductors is the chalcopyrite structure with space group I4¯2d. Density functional calculations are carried out within the local density approximation and generalized gradient approximation. The calculated lattice constant values are in good agreement with the available data. The electronic band structure shows that these chalcopyrite compounds are direct band gap semiconductors. To design a photovoltaic material with the band gap between 1.0 eV and 2.4 eV, indium (In) and gallium (Ga) are mixed to form CuInY2 (Y = S, Se, Te). It is observed that the energy band gap increases as the Ga concentration increases in CuIn1-xGaxY2 (Y = S, Se, Te). The computed optical parameters indicate that these materials can be the effective candidates for the solar cell devices. Phonon dispersion curves show that these compounds are dynamically stable. Moreover, the thermal properties, such as the entropy and the constant-volume specific heat are also calculated.	3.8	https://www.sciencedirect.com/science/article/abs/pii/S2352492820328014	2021
Dr. K. Iyakutti	Indian Journal of Physics	Investigation of optoelectronic properties of AgIn1−xGaxY2 (Y = Se, Te)	The electronic structure and optical properties of AgIn1−xGaxY2 (Y = Se, Te) are investigated using first-principles calculations based on density functional theory. Both the local density approximation (LDA) and generalized gradient approximation (GGA) are employed in the calculation. The crystal structure of ternary semiconductors is the tetragonal chalcopyrite structure with space group I4¯2d. The lattice parameters a(Å) and c(Å) are found to vary with the change in Ga composition. The energy gap across the Fermi level in the density of states plots shows that these materials are semiconductors. To compute accurate energy gap values, the LDA + U method is adopted. The calculated elastic constants indicate that these compounds are mechanically stable at normal pressure. The semiconducting nature of these materials may prove their applications in solar cells and photovoltaic absorbers. The optical parameters such as dielectric function, electron energy loss function, refractive index and reflectivity are computed.	2	https://link.springer.com/article/10.1007/s12648-021-02081-6#Ack1	2022
Dr. K. Iyakutti	Phase Transitions	Electronic structure, magnetic, optical and transport properties of half-Heusler alloys RhFeZ(Z=P, As, Sb, Sn, Si, Ge, Ga, In, Al) – a DFT study	The properties such as structural, mechanical, electronic structure, magnetic, optical and transport properties of the half-Heusler alloys of Rhodium RhFeZ(Z = P, As, Sb, Sn, Si, Ge, Ga, In, Al) are investigated at normal pressure. The alloys RhFeSb, RhFeSn, RhFeGe, RhFeGa, RhFeIn and RhFeAl are more stable in γ-phase. But the alloys RhFeP, RhFeAs and RhFeSi exhibit stability in β-phase under normal pressure. Among the investigated alloys, RhFeSn and RhFeGe are half-metallic at normal pressure. All the other half-Heusler alloys, RhFeP, RhFeAs, RhFeSb, RhFeSi, RhFeGa, RhFeIn and RhFeAl are ferromagnetic at normal pressure. To understand the transport properties, Seebeck coefficients, electrical conductivity, thermal conductivity and power factor are examined. The investigation infers that the alloys RhFeSn and RhFeGe possess remarkable transport properties and find potential applications in thermoelectric devices.	1.6	https://www.tandfonline.com/doi/abs/10.1080/01411594.2021.1944626	2021
Dr. K. Iyakutti	ACTA PHYSICA POLONICA A	Electronic Structure and Optical Properties of CsPbF3−yIy (y = 0, 1, 2) Cubic	The structural property, electronic structure and optical properties of lead-based halide perovskites CsPbF3−yIy (y = 0, 1, 2) are investigated. The computed electronic structure profile of CsPbF3−yIy (y = 0, 1, 2) reveals that these materials exhibit semiconducting behavior at normal pressure. The energy gap of CsPbF3 is tuned by substituting iodine atoms for fluorine atoms. The optical parameters, such as dielectric function, electron energy loss function, refractive index and reflectivity, are computed. The optical properties of these lead-based halide perovskites against the incident photon energy radiation indicate that these materials can be effective candidates for the solar cell applications.	0.7	http://przyrbwn.icm.edu.pl/APP/PDF/139/app139z6p11.pdf	2021

Dr. K. Iyakutti, Dr. V.J. Surya	Computational Condensed Matter	Effects of nanostructures on the hydrogen storage properties of MgH2 - A first principles study	Hydrogen storing properties of nanostructured MgH2 in two phases are investigated through first principles study using density functional theory. It is shown computationally that the hydrogen storage properties of MgH2 are significantly enhanced by proper engineering of the nanostructure. The nanoparticle clusters of MgH2 show linear behavior in adsorbing the hydrogen molecules and the binding energy values lie in the range −0.12eV to - 0.15eV. The MgH2 nanowires show non-linearity in hydrogen adsorption. For certain configuration, the hydrogen molecules binding energy values lie in the useful range (−0.15eV –> −0.27eV). Over all, the nanostructured MgH2 exhibits good hydrogenation and reduced desorption temperature. Selected configuration of the light metal free standing hydride MgH2 nanostructure, theoretically shows high hydrogen storage capacity which with suitable substrate is bound to reduce to the useful range of 6.4–8.8 wt%.	2.1	https://www.sciencedirect.com/science/article/abs/pii/S2352214322000053	2022
Dr. K. Iyakutti	Materials Science in Semiconductor Processing	First principles study of Co and Ni based half Heusler alloys	The structural stability, electronic structure, mechanical, magnetic and thermal properties of Co and Ni based half-Heusler (HH) alloys are studied. The most stable phase for CoCrSb, NiCrSb, NiCrBi, CoMnSb, CoMnBi and CoCrBi alloys is found to be γ-phase, whereas α-phase is the most stable phase for NiMnBi and NiMnSb among the three different phases (α, β, γ). As the pressure is increased, structural phase transition from γ-phase to α-phase is predicted for NiCrSb, CoCrBi, NiCrBi, CoMnBi, γ-phase to β-phase for CoMnSb and α-phase to β-phase for NiMnSb, at the pressures of 66.96 GPa, 16.91 GPa, 92.50 GPa, 14.58 GPa, 79.23 GPa and 71.47 GPa respectively. Density of states plot shows that there is no energy gap in spin-up state of all these HH alloys and in the spin-down state, the valence and conduction states are separated by a semiconducting energy gap. Thus, these compounds are half metallic. The spin polarized calculations predicted that these Heusler alloys are ferromagnetic nature. The total magnetic moment per unit cell (μcell) is found to be closer to the integer value of 2 μB, 3 μB and 4 μB. The 100% spin polarization at EF confirms the half-metallic nature of these materials. The dynamical stability of novel HH alloys has also been investigated by computing phonon density of states and it shows that these alloys (except CoCrBi and CoMnBi) are dynamically stable.	4.1	https://www.sciencedirect.com/science/article/pii/S1369800122004450?casa_token=f1r-jQBfWtcAAAA:dcnojRomaWI7HRtIIkD0f64N2DzZSGfITAQ9_Sn5pMoJBazjtiHdf_gdBWm08lLPDI1p7QoNOQ	2022
Dr. K. Iyakutti, Dr. V.J. Surya	Journal of Applied Mathematics and Computation,	Angular Momentum and Orbital Degrees of Freedom of s Electrons in an Atom—A New Quantum Theoretical Insight	Assigning dimension to θ on par with r, in the wave function Ψ(r,θ), we have quantum engineered the orbital angular momentum and the corresponding orbital degrees of freedom of s electrons. The quantized orbital angular momentum of s electron in an atom is estimated as 0.75ħ2 using angular momentum engineering. This restoration of orbital angular momentum leads to new additional quantum numbers to s electrons and there is a possibility for the alteration of s electron occupation. This newly discovered s electron property can be invoked where ever the present quantum theory is inadequate to explain some of the exotic properties observed in modern materials.	**	https://wap.hillpublisher.com/UpFile/202211/20221103172712.pdf	2022
Dr. K. Iyakutti, Dr. V.J. Surya	International Journal of Quantum Chemistry	Computational study of van der Waals interaction at the sub-nanometer scale and its influence on the molecular behavior under confinement conditions in graphene-2D h-BN heterostructure		2.2	https://onlinelibrary.wiley.com/doi/abs/10.1002/qua.27205	2023

Dr. K. Iyakutti	Indian Journal of Physics	Density functional study on electronic structure, magnetic and thermodynamic properties of YX’CrZ (X’ = Fe, Co; Z = As, Sb) quaternary Heusler alloys.	In this work, the first principles calculations are performed to analyze the electronic structure and magnetic properties of YX’CrZ (X’ = Fe, Co; Z = As, Sb) quaternary Heusler compounds based on density functional theory as implemented in the Vienna Ab initio Simulation Package (VASP). Among α, β and γ phases of the ordered LiMgPdSn structure, γ phase is found to be the most suitable stable structure. The electronic structure predicted that these alloys are half metallic. The energy gap values of YFeCrAs and YFeCrSb alloys are computed as 0.856 eV and 0.610 eV in the spin up state only and there is no energy gap in the spin down state. In YCoCrAs and YCoCrSb, the energy gap values of 0.516 eV and 0.854 eV are observed in the spin-down state. The computed ground state energy values of ferromagnetic and non-magnetic states show that these compounds are ferromagnetic. The magnetic moment values for YFeCrAs, YFeCrSb, YCoCrAs and YCoCrSb are computed as 4.087 µB, 4.007 µB, 5.042 µB and 5.064 µB respectively. The spin polarization is found to be 100%. Hence, these alloys may be used in spintronics. The phonon band structure calculations predicted that these compounds are dynamically stable	2	https://link.springer.com/article/10.1007/s12648-023-02904-8#Ack1	2023
Dr. K. Iyakutti	Physica B: Condensed Matter	Structural, electronic, magnetic, optical and thermoelectric properties of full-Heusler alloys Rh2FeZ (Z=Al, Ga, In): First principles calculations with GGA and GGA+U	The density functional theory was employed to explore the structural, electronic, magnetic, optical, and thermoelectric properties of full Heusler alloys Rh2FeZ (Z = Al, Ga, In). The structural properties of the alloys were investigated, and it was found that the Rh2FeZ (Z = Al, Ga, In) alloys are ferromagnetically stable in the Cu2MnAl type crystal structure. The dynamic stability was also evaluated using the phonon dispersion curve. The exchange correlation potential has been approximated using GGA and GGA + U methods. The electronic structure, density of states and magnetism for the GGA + U method show that all these alloys are indirect band gap semiconductor with half metallic ferromagnetic character. The total magnetic moment values of these alloys in GGA + U satisfy the Slater-Pauling (SP) rule. The dielectric function, refractive indices, and energy loss function are calculated optical properties. The Seebeck coefficients, electrical conductivity, thermal conductivity, and power factor as a function of temperature are calculated using the semi-classical Boltzmann transport theory to understand their thermoelectric properties. All of these results imply that full Heusler alloys composed of Rh2FeAl, Rh2FeGa, and Rh2FeIn would be good for spintronic and thermoelectric device applications.	2.8	https://www.sciencedirect.com/science/article/abs/pii/S0921452624000826	2024
Dr. K. Iyakutti	Chinese Journal of Physics	Ab-initio study of electronic and optical properties of Zr2NiZ (Z=Al, Ga, In) full Heusler alloys	The half-metallic property of Zr2NiZ (Z=Al, Ga, In) Heusler alloys with the Hg2CuTi-type structure has been studied. In Zr2NiZ (Z=Al, Ga, In) Heusler alloys, it is found that spin up states are metallic and spin down states have the semiconducting band gaps. It shows that these Heusler alloys are half-metallic. From the band structure of spin down state, it is observed that these alloys have the indirect band gap. The non-spin polarised and spin polarized calculations predicted that the ferromagnetic ground state energy is less than the non- magnetic ground state energy which shows that these alloys are ferromagnetic in nature. The total magnetic moments of the Zr2NiZ alloys are calculated to be around 3.0 µB for these Zr2NiZ (Z=Al, Ga, In) Heusler alloys. These alloys obey Slater Pauling rule µt = Zt −18. The optical properties like dielectric function, refractive index, energy loss function, reflectivity and absorption coefficient and extinction coefficients are computed for the first time. For spintronic devices, these alloys may be suitable.	5	https://www.sciencedirect.com/science/article/abs/pii/S0577907324000145	2024

Bharathi P, Harish S. Mathankumar G, Krishna Mohan M, Archana J, Kamalakannan S, Prakash M, Shimomura M, Navaneethan M.	Applied Surface Science	Solution processed edge activated Ni-MoS2 nanosheets for highly sensitive room temperature NO2 gas sensor applications	In this work, we report the effect of nickel incorporation into MoS2 nanosheets for room temperature sensing of NO2 gas. Interestingly, the concentration of Ni (3, 5, 7 at.%) ions plays a vital role in enhancing the morphological and optical properties. The increased edge active sites in nickel incorporated samples play a vital role in high-performance gas sensing. 7 at.% of Ni incorporated MoS2 showed 115% enhancement for 200 ppm of NO2 gas molecules at room temperature, compared to pristine and other concentrations of Ni-incorporated sensors. The enhancement in the gas sensing performance was explained by the possible mechanism. In addition to this, the first principle calculations were performed to identify the influence of Ni-atom into the MoS2 matrix. The electronic structure of the material was tuned by the incorporation of Ni-atom into the MoS2. This was confirmed from electronic band structure, PDOS, electron density difference and Bader charge transfer analyses.	6.7	https://doi.org/10.1016/j.apsusc.2022.154086	2022
Kamarajar Prakash, Santhanakrishnan Harish, Shanmugasundaram Kamalakannan, Thirumalaisamy Logu, Masaru Shimomura, Jayaram Archana, Mani Navaneethan	Journal of Energy Chemistry	Perspective on ultrathin layered Ni-doped MoS2 hybrid nanostructures for the enhancement of electrochemical properties in supercapacitors	Over the last two decades, extensive study has been done on two-dimensional Molybdenum Sulphide (MoS2) due to its outstanding features in energy storage applications. Although MoS 2 has a lot of active sulphur edges, the presence of inactive surfaces leads to limit conductivity and efficiency. Hence, in this article, we aimed to promote the additional active sites by doping various weight percentages (2%, 4%, 6%, 8% and 10%) of Nickel (Ni) into the MoS 2 matrix by simple hydrothermal technique, and their doping effects were investigated with the help of Physio-chemical analyses. X-ray diffraction (XRD) pattern, Raman, and chemical composition (XPS) analyses were used to confirm the Ni incorporation in MoS 2 nanosheets. Microscopic investigations demonstrated that Ni-doped MoS2 nanosheets were vertically aligned with enhanced interlayer spacing. Cyclic voltammetry, Galvanostatic charge–discharge, and electrochemical impedance spectroscopy investigations were used to characterize the electrochemical characteristics. The 6% Ni-doped MoS 2 electrode material showed better CSP of 528.7 F/g @ 1 A/g and excellent electrochemical stability (85% of capacitance retention after 10,000 cycles at 5 A/g) compared to other electrode materials. Furthermore, the solid-state asymmetric supercapacitor was assembled using Ni-doped MoS2 and graphite as anode and cathode materials and analysed the electrochemical properties in the two-electrode system. To determine the impact of the Ni-atom on the MoS 2 surface, first-principles computations were performed. Further, it was examined for electronic band structure, the projected density of states (PDOS) and Bader charge transfer analyses.	13.1	https://doi.org/10.1016/j.jechem.2023.01.002	2022
G Mathankumar, S Harish, M Krishna Mohan, P Bharathi, S Kamala Kannan, J Archana, M Navaneethan	Sensors and Actuators B: Chemical	Enhanced selectivity and ultra-fast detection of NO2 gas sensor via Ag modified WO3 nanostructures for gas sensing applications	Recently, nanostructured tungsten oxide-based materials have received much attention in the field of the gas sensor due to their superior size-dependent gas adsorption and catalytic properties. Herewith, we have successfully prepared pure and Ag-doped WO3 nanostructures via a hydrothermal method. The effect of doping (Ag) in WO3 and their gas sensing properties was systematically studied. Interestingly, the Ag-2 sensor revealed the enhanced gas sensing response of 52404% @1000 ppb, which is 5-fold higher than that of the pure WO3 sample at 150 . Moreover, Ag-2 sensor possessed an ultra-fast response and recovery time of 1 s and 3.5 s. Further, as prepared sensors exhibit excellent selectivity, repeatability, and long-term stability. In addition, the DFT calculations were performed to evaluate the adsorption and charge transfer dynamics of NH3, H2S, and NO2 gas molecules on pure and Ag-doped WO3 surfaces. These results pave the new pathway to developing real-time metal oxide-based gas sensors at lower operating temperatures.	8.4	https://doi.org/10.1016/j.snb.2023.133374	2023

Joseph Dona, J Archana, S Kamalakannan, M Prakash, K Hara, S Harish, M Navaneethan	Journal of Alloys and Compounds	Double charge polarity switching in Sb-doped SnSe for enhanced thermo-electric power generation	The pristine and antimony (Sb) doped tin selenide (SnSe) has been prepared by vacuum melting followed by ball milling process. The crystallographic pattern of both doped and undoped samples shows the formation of orthorhombic SnSe without any impurities. The influence of Sb on SnSe were confirmed from Projected Density of States (PDOS) and electron density analysis. The Elemental Probe Micro Analyzer (EPMA) technic used to confirm the presence of Sn, Se and Sb elements along with homogenous distribution. HR-TEM micrographs reveal highly crystalline nature of the samples as well as the formation of defects and distinguishable grains and grain boundaries, which helps to reduce the thermal conductivity of 10 wt% Sb doped SnSe samples to 0.55 W/mK at 600 K. Seebeck coefficient analysis has been discloses the double charge polarity switching in Sb substituted samples. Thus, 10 wt% Sb doped SnSe samples achieved a comparable negative Seebeck coefficient with respect to pristine SnSe, which can be a breakthrough in thermoelectric devices.	6.2	https://doi.org/10.1016/j.jallcom.2021.163269	2023
M Arockia Jenisha, S Kavirajan, S Harish, S Kamalakannan, J Archana, E Senthil Kumar, Naoki Wakiya, M Navaneethan	Journal of Colloid and Interface Science	Multiple approaches of band engineering and mass fluctuation of solution-processed n-type Re-doped MoS2 nanosheets for enhanced thermoelectric power factor	The thermoelectric (TE) performance of Molybdenum disulpide (MoS2) can be improved by the incorporation of nanomaterials. MoS2 has been reported as promising thermoelectric materials due to their large bandgap and low thermal conductivity. In the present work, n-type MoS2 was successfully synthesized by facile hydrothermal route with an excellent thermoelectric performance by introducing rhenium (Re) dopant. The structural and morphological analyses confirmed the incorporation of Re into Mo (Molybdenum) lattice. The thermoelectric results showed that both the electrical conductivity (σ) and Seebeck coefficient (S) has been increased with the increase in Re content (2.5, 5, 7.5 and 10 at%) and temperature (303 K to 700 K), while the thermal conductivity (κ) was low. Doping with Re on MoS2 enhances the electrical conductivity through band engineering, improving carrier concentration and shifting the Fermi level to the conduction band. Introducing a heavy atomic element can reduce the total thermal conductivity by facilitating mass fluctuation. The maximum Seebeck coefficient was obtained as 100 µVK 1 at 500 K for Re 5 at% sample, which is 3.7 times greater than undoped MoS2. In addition, introducing electrons through Re doping induced bipolar conduction. These enhancements have increased the power factor of 8 µWm-1K 2 at 650 K.	9.9	https://doi.org/10.1016/j.jcis.2023.08.201	2024

D Simon Patrick, P Bharathi, S Kamalakannan, J Archana, M Navaneethan, M Krishna Mohan	Applied Surface Science	Confined oxidation of 2D WS2 nanosheets forming WO3/WS2 nanocomposites for room temperature NO2 gas sensing application	In this article, we synthesized WO3/WS2 nanocomposites by facile hydrothermal synthesis followed by thermal annealing treatment and analysed its gas sensing properties. The thermal annealing process was carried out in different temperatures from 400 °C to 600 °C to form WO3/WS2 nanocomposite. During the thermal annealing process, the hydrothermally synthesized pure WS2 nanosheets undergo partial oxidation constructing WO3 on the surface developing active heterojunctions leading to increment in the sensing performance. The fabricated WO3/ WS2 samples showed superior sensitivity and selectivity towards NO2 gas molecules. The pristine WS2 nanosheets showed a response of 26% towards 10 ppm of NO2 gas with a response and recovery time of 13 s /18 s, whereas WO3/WS2 nanocomposite prepared by annealing at 600 °C showed a maximum response of around 123% with a short response time of 11 s and recovery time of 163 s. The DFT calculations were performed to understand the gas sensing performance and interfacial charge transfer between the WO3/WS2 nanocomposite and gas mole- cules. Therefore, this study demonstrates that the indigenous heterojunctions contribute extensively to improving the gas detection capabilities of WO3/WS2 nanocomposites at room temperature.	6.7	https://doi.org/10.1016/j.apsusc.2023.158554	2024
S Priyadharshini, V Vijay, S Kamalakannan, J Archana, M Navaneethan	Applied Physics Letters	Realizing an ultralow thermal conductivity via interfacial scattering and rational-electronic band reformation in p-type Mg3Sb2	Eco-friendly Magnesium antimonide (Mg3 Sb 2) has been extensively investigated as a promising and low-toxic thermoelectric material for intermediate (500–900 K) thermoelectric applications. Herein, p-type Zn-incorporated Mg3 Sb2 was prepared by hot press technique, and its thermoelectric transport properties were investigated. The formation of Mg3⍰x Znx Sb2 solid-solution plays a significant role in enhancing electrical conductivity of 34.59 S cm⍰1 due to the increased carrier concentration and reduced energy gap. Reduction in lattice thermal conductivity of 0.46 W m⍰1 K⍰1 at 753 K was obtained for Mg 3⍰x Znx Sb2 (x ¼ 0.15) by combined scattering effect of dislocations, lattice strain, and interfaces, which is clearly seen in HR-TEM and strain analysis. These favorable conditions lead to an enhanced thermoelectric figure-of-merit (zT) of 0.25 at 753 K, which is 400% improved compared to the pure Mg 3 Sb2 sample.	4	https://doi.org/10.1063/5.0180722	2024

M. Arockia Jenisha, S. Kavirajan, S. Harish, C. Kanagaraj, E. Senthil Kumar, J. Archana, N. Wakiya, M. Navaneethan	Emergent Materials	Coupling of band shift and phase transition for enhanced electrical conductivity in p-type metallic CuS towards mid-temperature thermoelectric application	Multiphase chalcogenides are highly interested candidate in thermoelectric application due to their unique band structure, which enhances electrical conductivity. Even though copper sulfide is a widely reported material for hermoelectrics, there have been no reports addressing its various densification methods to study thermoelectric behavior. This report represents the first promising study aimed at investigating the thermoelectric properties of copper sulfide using different densification methods. Herein, we prepared a multiphase ($Cu_{1.96}S$ + CuS) sample using the hydrothermal method followed by the hot press technique and compared its thermoelectric properties with single-phase ($Cu_{1.81}S$) sample prepared by the cold press method. XRD confirms the formation of multiphase ($Cu_{1.96}S$ + CuS), and TG/DTA shows the phase transition temperature at which the hot press has been carried out. The multiphase sample exhibits a maximum electrical conductivity of 180 $S cm^{-1}$ at 653 K, which represents a 55% improvement compared to the single-phase sample. This enhancement is a consequence of the high carrier concentration within the mixed phases, resulting in a gradual shift of the valence band towards the Fermi level (E_F). Notably, the multiphase sample has exhibited lower thermal conductivity than the single-phase sample, mainly due to the interface phonon scattering. Consequently, the zT value of the multiphase sample has increased to 0.5 at 753 K. The results of our study highlight the effectiveness of a simple hot-press technique process in enhancing the performance of thermoelectric materials. This discovery presents a practical and efficient approach for significantly enhancing the thermoelectric properties.	3.8	https://doi.org/10.1007/s42247-023-00597-7.	2024
Shinde Nikhil Dhanaji	Agrigenomics for Food and H	superTranscriptomic appr	Description of the subject. Analyzing transcriptomic data mainly relies on the availability of re	International	https://agrigenomicscongress.com/	2024
Shinde Nikhil Dhanaji	Journal of molecular evolutio	Unveiling the Genomic Sy	Sweet sorghum has gained global significance as a versatile crop for food, fodder, andbiofuel.	3.9	https://link.sp	Under Review
Varathan E	Separation and Purification Technology	Experimental investigation into the π-conjugated HT-g-C_3N_4/MoS_2 (X) evokes the electron transport in type-II heterojunction to achieve high photocatalytic antibiotic removal under visible-light irradiation	Antibiotics have been recently discovered in the aquatic environment, generating significant concerns. It is critical to create visible light semiconductor photocatalysts with high catalytic activity to use sunlight for antibiotic degradation.	12.7	https://doi.org/10.1016/j.seppur.2022.121028	2022
Varathan E	Dalton Trans	Chemical bonding in actinyl(V/VI) dipyriamethyrin complexes for the actinide series from americium to californium: a computational investigation	The separation of minor actinides in their dioxocation (i.e., actinyl) form in high-valence oxidation states requires efficient ligands for their complexation. In this work, we evaluate the complexation properties of actinyls including americyl, curyl, berkelyl, and californyl in their pentavalent and hexavalent oxidation states with the dipyriamethyrin ligand (L) using density functional theory calculations.	4	10.1039/d2dt01142e	2022

Varathan E	Phys. Chem. Chem. Phys	Why trans and not cis? – Molecular dynamics and DFT study on selective separation of dihaloethene isomers using perethylated pillar[5]arene†	From this work, one can understand why only trans dihaloethenes are encapsulated while cisdihaloethenes are not.	3.3	10.1039/d2cp02367a	2022
Varathan E	Organic & Biomolecular Chemistry	Iodo-sulphonylation of 1,6-enynones: a metal-free strategy to synthesize N-substituted succinimides	An iodine-mediated radical cyclization of 1,6-enynones with sulphonyl hydrazides using tert-butyl hydroperoxide (TBHP) as the oxidant has been developed for the synthesis of iodo-sulphonylated-succinimide derivatives.	3.2	10.1039/d2ob01277d	2022
Varathan E	New J. Chem.	Design and development of imidazo[4,5-f] [1,10] phenanthroline-Zn(II) based fluorescent probes for specific recognition of ATP with tunable optical responses and probing the enzymatic hydrolysis of ATP by alkaline phosphatase	The development of chemosensors for the selective detection of specific biologically important analytes continues to be of great attention in contemporary analytical chemistry. Among the several biologically important analytes, selective detection of adenosine 50-triphosphate (ATP), is extremely crucial as this is considered as a primary energy source of all living organisms, and responsible for intracellular energy transfer that in turn controls several cellular functions.	3.59	10.1039/d2nj04704g	2022
Varathan E	Langmuir	Investigation of Guest-Induced Flexibility in Pyrazine Derivative of ALFFIVE MOF via Molecular Simulation	One of the important understandings of porous solids like metal−organic frameworks (MOFs) is their flexibility. Therefore, there are certain computational studies on flexible MOFs in the literature, primarily concentrating on MIL-53, UiO-66, and DUT-49. Here, investigation of another class of MOF, that is, [Ni(1,4-pyrazine)2(AlF5)]n, was shown to have guestinduced flexible characteristics; nevertheless, the mechanism for the emergence of flexibility is uncertain.	4.3	https://doi.org/10.1021/acs.langmuir.2c02027	2023
Varathan E	Colloids and Surfaces A: Physicochemical and Engineering Aspects	Molecular interaction and corrosion inhibition of benzophenone and its derivative on mild steel in 1 N HCl: Electrochemical, DFT and MD simulation studies	In this study, Benzophenone (BP) and 2-Aminobenzophenone (2-A.BP) were evaluated for the corrosion inhibition effect on mild steel in 1 N HCl solution with various temperatures ranging from 303 to 333 K using gravimetric analysis.	5.2	https://doi.org/10.1016/j.colsurfa.2023.130919	2023
Varathan E	Journal of Molecular Structure	Supramolecular cocrystals of dispiro-P3N3-dicarboxylic acid: Synthesis, structural characterization and hirshfeld surface analysis	The design of cocrystals for a particular molecule begins with examining that molecule’s functional group and selecting a complementary functional group that would generate the foreseeable supramolecular synthons. In this work, the cyclotriphosphazene-based compound Dispiro-P3N3-dicarboxylic acid (L) was identified to produce two cocrystals with two different N-donor compounds such as 4,4’ -bipyridine and piperazine by slow evaporation technique.	3.8	https://doi.org/10.1016/j.molstruc.2023.135888	2023

Varathan E	ACS Omega	Polarity-Induced Morphological Transformation with Tunable Optical Output of Terpyridine−Phenanthro[9,10 d]imidazole-Based Ligand and Its Zn(II) Complexes with I−V Characteristics	we have designed and synthesized a functional π-conjugated molecule (TP) having phenanthro[9,10-d]imidazole with terpyridine substitution at the 2 position and its corresponding metal complexes (TPZn and (TP)2Zn). By varying the polarity of the self-assembly medium, TP, TPZn, and (TP)2Zn are fabricated into well-ordered superstructures with morphological individualities.	4.1	https://doi.org/10.1021/acsomega.3c06283	2023
Varathan E	Journal of Environmental Chemical Engineering	Bifunctional properties of Acacia concinna pod as a natural surfactant-based eco-friendly benign corrosion inhibitor towards carbon steel protection in saline medium: Experimental and theoretical research	A facile approach has been targeted in combating both the electrochemical and microbial-induced corrosion (MIC) using an eco-friendly surfactant-based plant extract, Acacia concinna pod extract (AcPE) as a corrosion inhibitor for carbon steel (CS) in saline medium (3.5% NaCl). The ethanolic extract from the pod of Acacia concinna was found to contain glycidyl oleate, a fatty acid-based phytochemical, analysed by Gas Chromatography-Mass Spectrometry (GC-MS) showed the dual inhibitory effect.	8.2	https://doi.org/10.1016/j.jece.2024.111947	2024
Sharma, Ridhi, Dhananjay Jade, Surender Mohan, Rahul Chandel, and Shobana Sugumar	Journal of Biomolecular Structure and Dynamics	In-silico virtual screening for identification of potent inhibitor for L2-β-lactamase from Stenotrophomonas maltophilia	Stenotrophomonas maltophilia, a Multiple-Drug-Resistant proteobacterium found in healthy normal flora and fauna with an aerobic and non-fermentative respiratory process, is majorly involved in Healthcare-Associated Infections (HAI). The Multiple-Drug-Resistance takes place by secretion of the β-Lactamase enzyme, which hydrolyzes the β-Lactam antibiotics and currently serving as a significant clinical challenge by substantially effecting the mortality rate. In this study, involved 2D Similarity, Molecular docking, and Molecular Simulation for the commercially available ZINC database compounds to overcome this resistance mechanism and find out a proper potent inhibitor for the target L2-β-Lactamase, which would not get cleaved by the hydrolytic activity of the L2-β-Lactamase natural enzyme.	β-Lactamase potent inhibitors for S. maltophilia.	https://www.tandfonline.com/doi/abs/10.1080/07391102.2020.1805365	2021
Chandela, Rahul, Dhananjay Jade, Surender Mohan, Ridhi Sharma, and Shobana Sugumar	Combinatorial Chemistry & High Throughput Screening	Identification of Therapeutic Drug Target of Stenotrophomonas maltophilia Through Subtractive Genomic Approach and in-silico Screening Based on 2D Similarity Filtration and Molecular Dynamic Simulation	To find out the drug target and a novel inhibitor for Stenotrophomonas maltophilia.	Novel inhibitors against S.maltophilia	https://www.ingentaconnect.com/content/ben/cchts/2022/00000025/00000001/art00015	2022
Sreenithya K. H, Dhananjay Jade, Michael A. Harrison & Shobana Sugumar	Journal of Molecular Modeling	Identification of natural inhibitor against L1 β-lactamase present in Stenotrophomonas maltophilia	Virtual screening, molecular docking, and dynamic simulation methods are followed to get the best inhibitor for L1 β-lactamase.	This compound can act as a potent natural inhibitor for L1 β-lactamase.	https://link.springer.com/article/10.1007/s00894-022-05336-z	2022

Himaja Kuppachi	Journal of Biomolecular Structure and Dynamics	Aromatase inhibitors identified from Saraca asoca to treat infertility in women with polycystic ovary syndrome via in silico and in vivo studies	Polycystic ovary syndrome (PCOS) is a widely occurring metabolic disorder causing infertility in 70%–80% of the affected women. Saraca asoca, an ancient medicinal herb, has been shown to have therapeutic effects against infertility and hormonal imbalance in women. This study was aimed to identify new aromatase inhibitors from S. asoca as an alternative to the commercially available ones via in silico and in vivo approaches. For this, 10 previously reported flavonoids from S. asoca were chosen and the pharmacodynamic and pharmacokinetic properties were predicted using tools like Autodock Vina, GROMACS, Gaussian and ADMETLab. Of the 10, procyanidin B2 and luteolin showed better interaction with higher binding energy when docked against aromatase (3S79) as compared to the commercial inhibitor letrozole. These two compounds showed higher stability in molecular dynamic simulations performed for 100 ns. Molecular mechanics Poisson–Boltzmann surface analysis indicated that these compounds have binding free energy similar to the commercial inhibitor, highlighting their great affinity for aromatase. Density functional theory analysis revealed that both compounds have a good energy gap, and ADMET prediction exhibited the drug-likeness of the two compounds. A dose-dependent administration of these two compounds on zebrafish revealed that both the compounds, at a lower concentration of 50 µg/ml, significantly reduced the aromatase concentration in the ovarian tissues as compared to the untreated control. Collectively, the in silico and in vivo findings recommend that procyanidin B2 and luteolin could be used as potential aromatase inhibitors for overcoming infertility in PCOS patients with estrogen dominance.	Impact factor- 4.4 , Scopus-Q1	https://www.tandfonline.com/doi/full/10.1080/07391102.2024.2310793	2024
Himaja Kuppachi	Journal of Applied Pharmaceutical Science	In-silico screening of potential anti-androgenic and anti-estrogenic phytocompounds from Saraca asoca for polycystic ovary syndrome treatment	Saraca asoca (Roxb.) Willd. [Family: Fabaceae (Caesalpiniaceae)], commonly known as Ashoka, is a medicinal plant used for many gynaecological disorders, including polycystic ovary syndrome (PCOS). PCOS is a common gynaecological disorder affecting the ovarian steroidogenesis pathway, leading to hormonal imbalance. In this study, 56 ligands reported from S. asoca were selected and computationally analyzed for their binding affinity to the targets from the ovarian steroidogenesis pathway- aromatase, 17beta-hydroxysteroid dehydrogenase type 1 (17β-HSD1), androgen, and estrogen receptors (α and β). Molecular docking was performed by Autodock Vina, density functional theory (DFT) was performed by Gaussian software, and absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties were checked using ADMETLab. Among the 56 compounds, higher docking scores were obtained for procyanidin B2 with−11.7 and −10.4 kcal/mol against aromatase and 17β-HSD1, respectively, and leucopelargonidin with −10 and −9.1 kcal/mol against androgen receptor and estrogen β receptor followed by epicatechin gallate, amyrin, procyanidin B1, leucocyanidin and ellagic acid. ADMETLab prediction showed that all the top seven compounds fulfilled the criteria for drug-likeness. DFT analysis showed improved chemical and biological reactivity with a substantial transfer of charge between electron-donor to electron-acceptor groups for all seven compounds. Here, we put forth procyanidin B2 and leucopelargonidin with high binding energy scores against aromatase and 17β-HSD1 as potential inhibitors of excess estrogen and testosterone biosynthesis in PCOS women.	Cite score: 2.4, SJR: 0.26	https://japsonline.com/abstract.php?article_id=4162&sts=2	2024

Dr. V. J. Surya, Gobinath Marappan	Materials Letters	Naphthalene appended diketopyrrolopyrrole derivatives functionalized on ZnO nanostructures: An investigation on gas adsorption induced surface potential changes at room temperature	ZnO nanostructures prepared at different pH (9 and 11) were functionalized with naphthalene appended diketopyrrolopyrrole derivatives with thiophene (TDPP) and phenyl (PDPP) functionals. The functionalization was ascertained through various characterization techniques like XRD, FESEM, UV-Visible absorption and PL studies. Gas adsorption-induced surface potential of functionalized samples were studied through scanning Kelvin probe system at room temperature in the presence of various volatile organic compounds (VOCs) like acetone, benzene, ethanol, nonanal, n-hexane, 1-hexanol and triethylamine (TEA). Interestingly, the functionalized ZnO nanostructures obtained at pH 9 showed ~1.5 times better response towards 1-hexanol when compared to the functionalized pH 11 ZnO counterparts. Density functional theory calculations revealed that the DPP derivatives showed higher binding affinity towards ethanol, 1-hexanol and nonanal. Overall, this combined experimental and computational studies suggested that the DPP derivatives functionalized ZnO nanostructures would be useful for detection of VOCs such as alcohols and aldehydes.		3	https://www.sciencedirect.com/science/article/abs/pii/S0167577X2101421X	2021
Dr. V. J. Surya, Rence P Reji, Gobinath Marappan	Materials Letters	VOCs adsorption induced surface potential changes on phthalocyanines: A combined experimental and theoretical approach towards food freshness monitoring	Many organic molecules such as porphyrins, pthalocyanines, pyrene ligands and so on are being used to detect volatile organic compounds (VOCs). The richness in π-electrons, coordination metals and their structural integrity make them as potential candidates for chemical sensing applications. In this work, metal free (H2Pc) and iron (II) phthalocyanines (FePc) are used for detecting VOCs such as 1-hexanol, nonanal, triethylamine and so on. The structural, morphological and optical properties of as deposited films of H2Pc and FePc on fluorine doped tin oxide substrates are characterized by XRD, HR-SEM, UV–Vis adsorption and Raman spectroscopy studies. Their gas adsorption properties are investigated through scanning Kelvin probe by means of change in contact potential difference in dark as well as light illumination conditions. Among both pthalocyanines, FePc shows highly selective response towards 1-hexanol under visible light exposure. Interestingly, the one to one molecular computations have revealed that FePc show higher interaction towards VOCs when compared to H2Pc. Overall, being a marker for food freshness monitoring, 1-hexanol can be detected using FePc based photo enhanced room temperature gas sensors.		3	https://www.sciencedirect.com/science/article/abs/pii/S0167577X21016438	2022
Dr. V. J. Surya, Rence P Reji, C B Sarath Kumar	ACS Applied Electronic Materials	Tuning the π Conjugation of 2 Thiohydantions toward a Rigorously Defined Detection of Volatile Organic Compounds by Surface Photovoltage	The design of portable devices by immobilization of sensory probes using donor−acceptor (D−A) architectures enables the visual detection and onsite analysis of volatile organic compounds (VOCs). In this work, we have reported on the synthesis of different D−A architectures of 2-thiohydantoin (2TH) derivatives by extending the conjugation with phenyl (Ph-2TH), naphthalene (Naptha-2TH), and anthracene (Anthra-2TH) moieties at the C5 position. Single-crystal X-ray analysis reveals that extending the conjugation leads to variation in the molecular arrangement in the crystal lattice. Ph-2TH and Naptha-2TH show ribbon-like self-assembled layered arrangements, whereas Anthra 2TH crystallized in herringbone packing in the crystal lattice. The C−S···H interactions were varied with interatomic distances of 2.67, 2.63, and 2.27 Å, respectively, for phenyl, naphthalene, and anthracene. The photophysical and excited-state gas-phase interactions using scanning kelvin probe studies reveal that 2TH ensembles alter their surface photovoltages toward recognition of different VOCs (like ethanol, acetone, toluene, triethylamine, nonanal, and chloroform) depending on their donor and acceptor nature. All three 2TH derivatives showed n-type behavior with high selectivity toward nonanal, and Anthra-2TH exhibited high response (91.02%) within 278 s as well as recovery (92.83%) in surface photovoltages in 647 s. Combined experimental and computational studies demonstrate that the aromatic moieties appended 2TH ensembles would be an efficient D−A ensemble for the detection of VOCs containing carbonyl and alcohol functionalities aiding strong intermolecular interactions.		4.7	https://pubs.acs.org/doi/abs/10.1021/acsaelm.2c00149	2022

Dr. V. J. Surya, Rence P Reji, C B Sarath Kumar, Gobinath Marappan	IOP Conference Series: Materials Science and Engineering	Hydration of amino acids: An investigation using density functional theory	Herein, we have investigated the effect of hydration of seven amino acids (AAs) such as alanine, aspartic acid,cysteine, glutamine, lysine, methionine, and phenylalanine with different number of water molecules using density functional theory. Among the hydrophobic AAs, cysteine has the highest interaction with water whereas in hydrophilic AAs, aspartic acid has the highest interaction with water. With the increase in number of water molecules, it is noted that alanine forms the most stable complex with water and methionine+water complex has least stability.In addition, we have calculated the chemical descriptors like chemical potential, electronegativity, hardness, softness, electrophilicity index of AAs to validate their interaction with water molecules. Interestingly, the gas phase interaction energy results match with the trend of electrophilicity index valuesof AAs.	**	https://iopscience.iop.org/article/10.1088/1757-899X/1219/1/012006	2022
Dr. V. J. Surya, Rence P Reji, C B Sarath Kumar, Gobinath Marappan	Chemosphere	Hydration effect of selected atmospheric gases with finite water clusters: A quantum chemical investigation towards atmospheric implications	Water vapor in atmosphere is ubiquitous, and it varies according to geographical locations. Various toxic and non-toxic gases co-exist with water vapor/moisture in the atmosphere. This computational study addresses the fact that how those gases interact with water vapor. We have done quantum chemical density functional theory calculations to probe the interaction of certain gases with a finite number of water molecules in gas phase with various functionals/basis sets. An ensemble of 14 gas molecules comprising various diatomic, triatomic, and polyatomic gases have been chosen for the investigations. The intermolecular interactions are understood from the interaction energy, electrostatic potential, frontier molecular orbitals, energy gap, and natural bond orbital analyses. Furthermore, quantum molecular descriptors such as electronegativity, chemical potential, chemical hardness and electrophilicity index are calculated to have deep insight on chemical nature of the gas molecules. Additionally, we have done implicit solvent modelling using PCM, and the corresponding solvation energies have been calculated. Interestingly, all the calculations and analyses have projected the similar results that Cl2, SO2, and NH3 have very high interaction with the water clusters. To mimic various altitudes (0 km, 5 km and 10 km) in the atmosphere, thermochemistry calculations have been carried out at different temperature and pressure values. The Gibbs free energies of formation suggest that the hydration of Cl2 is higher followed by O2, SO2 and NH3 at all altitudes. Remarkably, it is found that the formation of hydrated clusters of Cl2 and O2 with 4H2O are thermodynamically favourable. On the other hand, SO2 and NH3 requires 5H2O and 3H2O to form thermody namically favourable clusters. In summary, it is anticipated that this kind of extensive computational studies facilitate to understand the structural, electronic, chemical and thermochemical properties of hydrated atmo spheric gases that leads to the formation of prenucleation clusters followed by atmospheric aerosols.	8.8	https://www.sciencedirect.com/science/article/abs/pii/S0045653522024407	2022
Dr. K. Iyakutti, Dr. V.J. Surya	Computational Condensed Matter	Effects of nanostructures on the hydrogen storage properties of MgH2 - A first principles study	Hydrogen storing properties of nanostructured MgH2 in two phases are investigated through first principles study using density functional theory. It is shown computationally that the hydrogen storage properties of MgH2 are significantly enhanced by proper engineering of the nanostructure. The nanoparticle clusters of MgH2 show linear behavior in adsorbing the hydrogen molecules and the binding energy values lie in the range −0.12eV to - 0.15eV. The MgH2 nanowires show non-linearity in hydrogen adsorption. For certain configuration, the hydrogen molecules binding energy values lie in the useful range (−0.15eV –> −0.27eV). Over all, the nanostructured MgH2 exhibits good hydrogenation and reduced desorption temperature. Selected configuration of the light metal free standing hydride MgH2 nanostructure, theoretically shows high hydrogen storage capacity which with suitable substrate is bound to reduce to the useful range of 6.4–8.8 wt%.	2.1	https://www.sciencedirect.com/science/article/abs/pii/S2352214322000053	2022

Dr. V. J. Surya, Rence P Reji	Small	Unprecedented Multifunctionality in Novel Monophase Micro/Nanostructured Ti-Zn Alloy	It is always challenging to integrate multiple functions into one material system. However, those materials/devices will address society's critical global challenges and technological demands if achieved with innovative design strategies and engineering. Here, one such material with a broader spectrum of desired properties appropriate for seven applications is identified and explored, and a glucose-sensing-triggered energy-storage mechanism is demonstrated. To date, the Titanium (Ti)-Zinc (Zn) binary alloys are investigated only as mixed phases and for a maximum of three applications. In contrast, the novel single phase of structurally stable 50 Ti-50 Zn (Ti0.5Zn0.5) is synthesized and proven suitable for seven emerging applications. Interestingly, it is thermally stable up to 750 °C and possesses excellent mechanical, tribological properties and corrosion resistance. While exceptional biocompatibility is evident even up to a concentration of 500 µg mL−1, the antibacterial activity against E. coli is also seen. Further, rapid detection and superior selectivity for glucose, along with supercabattery behavior, unambiguously demonstrate that this novel monophase is a remarkable multifunctional material than the existing mixed-phase Ti-Zn compounds. The coin-cell supercapacitor shows outstanding stability up to 30 000 cycles with >100% retention capacity. This allows us to prototype a glucose-sensing-triggered energy-storage-device system for wearable point-of-care diagnostic applications.	13.3	https://onlinelibrary.wiley.com/doi/abs/10.1002/smll.202305126	2023
Dr. V. J. Surya, Rence P Reji, C B Sarath Kumar, Gobinath Marappan	ACS Applied Nanomaterials	First-Principles Density Functional Theory Calculations on the Potential of Sc2CO2 MXene Nanosheets as a Dual-Mode Sensor for Detection of Volatile Organic Compounds in Exhaled Human Breath	Volatile organic compounds (VOCs), namely, acetone, ethanol, acetonitrile, 2-propanol, isoprene, and toluene exhaled in human breath act as potential biomarkers for the identification of certain physiological disorders. This work investigates the sensing capability of two-dimensional Sc2CO2 MXene nanosheets toward these VOCs using first-principles density functional theory calculations. Since carbon dioxide and water vapor persist in the exhaled breath, their interaction with Sc2CO2 as interferent species is examined too. It is found that 2-propanol (−0.63 eV), ethanol (−0.59 eV), and acetonitrile (−0.51 eV) show higher interaction with the Sc2CO2. Meanwhile, the chemiresistive sensorial behavior has been examined, and it is revealed that Sc2CO2 is highly sensitive to acetonitrile (50.20%). Both ethanol (1.03 × 10−3 s) and 2-propanol (5.24 × 10−3 s) have a fast recovery at room temperature. Alternatively, the change in work function of Sc2CO2 nanosheets on adsorption of VOC biomarkers has been examined. The corresponding results have proved that the work function-based Sc2CO2 sensor is sensitive to physisorbed species like toluene (47.62%) and isoprene (37.83%) that are not quantifiable using the chemiresistive sensing mechanism. Overall, our research predicts that the Sc2CO2 MXene nanosheet can be utilized as a dual-mode sensor to detect potential VOC biomarkers in the exhaled breath. Also, our results will assist the experimentalists in designing MXene nanosheet-based room-temperature sensors as point-of-care breathalyzers for disease diagnosis.	5.9	https://pubs.acs.org/doi/abs/10.1021/acsanm.2c05474	2023

Dr. V. J. Surya, M. Elakia, Rence P Reji, C B Sarath Kumar	International Journal of Computational Materials Science and Engineering	Adsorption Characteristics of Pristine and Defective SWCNTs towards F and Cl species: A Density Functional Theory Investigation Towards Water Quality Monitoring Applications	To keep drinking water safe and of high quality, levels of fluorine and chlorine must be continuously monitored. In this study, we have used density functional theory (DFT) simulations to evaluate the mono/di fluorine and chlorine sensing ability of pristine and defective armchair (5,5) and zigzag (10,0) single-walled carbon nanotubes (SWCNTs) in different sites and orientations. Water molecules are taken into consideration as co-adsorbents to assess their impact on the halogenated SWCNTs. Specifically, the potent chemisorption of F and the dissociative adsorption of F2 on armchair/zigzag single-walled carbon nanotubes (ASWCNTs/ZSWCNTs) indicate that CNTs may be useful in the desalination of water. According to the computed adsorption energies, Cl/Cl2 adsorbed on SWCNTs appears to be advantageous, which qualifies them as sensor candidates. Water interaction studies have shown that chlorinated SWCNTs have shown higher interaction with it when compared to fluorinated counterparts. Hence. water may act as a co-player to improve SWCNTs' ability to sense chlorine. Finally, it has been demonstrated by ab-initio molecular dynamics simulations that the co-adsorbed systems of water molecules and halogens are stable at ambient temperature. Overall, our results demonstrate that both ASWCNTs and ZSWCNTs can be used as room-temperature chlorine sensors for water quality monitoring applications.	1.3	https://www.worldscientific.com/doi/abs/10.1142/S2047684123500562	2023
Dr. V. J. Surya, Rence P Reji	RSC Molecular Systems Design & Engineering (MSDE)	A quantum chemical assessment on the sensing ability of porphyrins and phthalocyanines towards volatile organic compounds using density functional theory investigations	In this work, we have investigated the sensing ability of four organic semiconductors namely, H2TPPCOOH and ZnTPPCOOH porphyrins, H2Pc and FePc phthalocyanines for the detection of 16 different volatile organic compounds (VOCs) through first-principles density functional theory (DFT) calculations. We have calculated various electronic properties of VOCs and organic molecules such as HOMO–LUMO, dipole moment, and global reactivity descriptors. The reactivity of VOCs mainly depends on the LUMO and the orbital energy gap. Similarly, the prime descriptors that are needed for understanding the organic molecules are softness, electrophilicity, and HOMO values. Most of the VOCs are physisorbed on the organic molecules. Few VOCs like ammonia (−1.42 eV) and acetonitrile (−1.21 eV) are chemisorbed on FePc with strong adsorption energies. H2Pc has better adsorption to diethylene glycol (−0.24 eV). H2TPPCOOH and ZnTPPCOOH show good binding affinity towards ammonia (−0.42 and −0.50 eV). Furthermore, the chemiresistive sensing properties of the sensors have revealed that H2Pc is sensitive and selective towards diethylene glycol, a potential pollutant that causes renal failure. FePc is sensitive towards all 16 VOCs and hence, it can be used as a universal sensor. Also, it can be used as a single-time sensor due to its strong chemisorption towards VOCs. H2TPPCOOH is highly sensitive to triethylamine and ZnTPPCOOH has high sensitivity to ammonia. Both triethylamine and ammonia cause severe respiratory diseases. Being a powerful tool, the DFT investigations have yielded results that are well-matched with the previously reported experimental works. In summary, we believe that our computational investigations will be useful to build sensor devices composed of highly sensitive and selective porphyrins and phthalocyanines for sensing VOCs from various sources in and around us	3.6	https://pubs.rsc.org/en/content/articlelanding/2024/me/d3me00175j/unauth	2023

Dr. V. J. Surya, Gobinath Marappan	Surfaces and Interfaces	Response to VOCs stimuli by triphenylamine derivatives functionalized zinc oxide nanorods: A promising material for food freshness monitoring	In this work, we have examined the photo-induced volatile organic compounds (VOCs) sensing ability of triphenylamine (TPA) derivatives functionalized zinc oxide nanorods (ZnO NRs) using the scanning Kelvin probe (SKP). We have explored the effect of contact potential difference variance and surface photovoltage in both dark and visible light illumination under different VOCs with reference to the ambient conditions. The ZnO NRs are synthesized by hydrothermal method followed by functionalization with three different TPA organic molecules namely (i) 4-formyltriphenylamine-acetophenone, (ii) 4,4’-diformyltriphenylamine-acetophenone, and (iii) 4,4’,4’’-triformyltriphenylamine-acetophenone (TFTPA). The pure and functionalized ZnO NRs are characterized by XRD, FESEM, HR-TEM, UV-visible absorption spectroscopy, Raman spectroscopy, XPS, and, SKP system. Three different VOCs such as ethanol, nonanal, and triethylamine are exposed on pure and functionalized ZnO NRs. In dark condition, high surface potential changes have been observed for nonanal in all the samples. Noteworthy, TFTPA_ZnO NRs show high adsorption towards nonanal during visible light illumination too. The irradiation of light has tuned the energy levels favorable for enhanced charge transfer between nonanal and TFTPA_ZnO. In parallel, the VOCs adsorption mechanisms are understood through density functional theory calculations. The computational adsorption energy and Mulliken charge analysis results are in accordance with the experimental ones. Overall, this combined study suggests that the ZnO NRs functionalized with the TPA derivatives are highly sensitive to nonanal. This can be used to monitor the freshness of edible oils (Peanut, soybean, and linseed), virgin olive oil, yak meat, etc. under visible light illumination.	6.2	https://www.sciencedirect.com/science/article/pii/S2468023023010143	2024
D.Ramkumar	-/AFMD	DFT study on electronic properties of black phosphorene and Au decorated black phosphorene	https://docs.google.com/document/d/1OJYzduTdtPKRjTfqpLCS4e0T10_OU5vT/edit?usp=drive_link&ouid=108499878835570613663&rtpof=true&sd=true	-	https://docs.google.com/presentation/d/1y9ejk0ca3JzPzpArpxux75m75WpRpttJ/edit?usp=drive_link&ouid=108499878835570613663&rtpof=true&sd=true	2024
Veerapandiyan Kandasamy	Natural Product Research	De novo assembly and annotation of Caesalpinia bonducella L. seed transcriptome identifies key genes in the biosynthesis of bonducellin, a homoisoflavonoid	Caesalpinia bonducella L. is a traditional medicinal plant containing a potential homoisoflavonoid, bonducellin, with therapeutic values against polycystic ovary syndrome, oxidative damage, pathogenic bacteria, irregular menstrual cycle, ovarian cancer and diabetes. Owing to the multi-therapeutic properties of bonducellin, knowledge of its biosynthetic pathway genes will help understand its regulatory mechanism and thus improve the yield. This study sequenced C. bonducella seed mRNA transcriptome to identify the genes in bonducellin biosynthesis. Before this, the presence of bonducellin in the seed samples was analysed by HPLC using the chemically synthesised bonducellin as the standard. Seven key genes encoding enzymes involved in the synthesis of bonducellin via the phenylpropanoid pathway were identified. The expression of selective genes from the bonducellin biosynthetic pathway was validated using qRT-PCR and comparable with RNA-Seq data. Here, we put forth the sequences of 67,560 genes from C. bonducella and highlight the bonducellin biosynthetic pathway genes.	Impact Factor- 2.2, Q1	https://www.tandfonline.com/doi/full/10.1080/14786419.2024.2301740	2024

Veerapandiyan Kandasamy	Journal of microbiology, biotechnology and food sciences	In-silico screening of phytochemical compounds in Caesalpinia bonducella L. seeds against the gene targets of ovarian steroidogenisis pathway	Polycystic ovary syndrome (PCOS) is the most common gynaecological disorder among reproductive-age women. Impaired metabolism of androgens and estrogens is one of the leading causes of PCOS. In India, medicinal herbs are being explored for their anti-androgenic and anti-estrogenic properties. In this study, we have screened the seed extracts of the herbal plant, Caesalpinia bonducella for potent inhibitors of estrogen and testosterone biosynthesis and assimilation. Methanol extract of C. bonducella seed kernels were subjected to gas chromatography - mass spectrometry (GC-MS) to identify the phytochemical constituents. Out of forty-three phytochemical compounds identified from the extract, eight compounds were selected based on Lipinski's rule of five for molecular docking. The selected phytochemical compounds were docked against specific targets of ovarian steroidogenesis pathway; human aromatase (CYP19A1), human 17β-hydroxysteroid dehydrogenase type 1 (HSD17B1), human androgen receptor and estrogen receptor α. Further, the nature of these compounds was validated using density functional theory (DFT) calculations and ADME/T studies. As per the molecular docking output, compounds 33, 35, 38, 40, and 43 exhibited higher binding affinities against the four selected targets. Phytochemical compounds were optimized using Gaussian 16 with the B3LYP function and the 6-31G(d, p) basis set and were correlated with docking results. ADME/T helps in identifying the potential drug candidates from a pool of drugs. Five phytochemical compounds, 33, 35, 38, 40, and 43 were found to have the ability to bind and inhibit appropriate targets in the ovarian steroidogenesis pathway. Hence, these compounds can be further characterized in vitro and in vivo for alleviating PCOS.	Impact Factor-0.9, Q3	https://office2.jmbfs.org/index.php/JMBFS/article/view/6124	2023
Greeshma R	Pramana	Tuning electronic and magnetic properties of FeRh alloy by chemical and physical method	The electronic, magnetic and thermodynamic properties of ordered and chemically disordered FeRh alloy are studied using ab-initio methods. The equiatomic FeRh composition is reported for both ordered and disordered phases. Chemically disordered FeRh is reported and the effect of disorder on electronic and magnetic properties is discussed. Further, we have reported the effects of stress and strain in both the ordered and disordered phases. The result is only for the cubic phase, and no distortion has been taken into consideration. This study is motivated by the recent resurgence in the FeRh and is inspired by the fact that it is possible to sustain the barocaloric properties over the cycle. Hence, we have discussed the properties of FeRh with chemical disorder and pressure simultaneously to gain an insight into the compound effect and the interplay between them.	2.8		2023
Yashdeep Podder	Sci-Connect Poster Presentation	DATA ANALYSIS AND PREDICTION OF METAL TRIHALIDE PROPERTIES USING STRUCTURAL AND STRUCTURAL AND THERMODYNAMIC FINGERPRINTS	The quantum mechanical calculations aided by powerful supercomputers and experiments has resulted in a wealth of data for materials. This has widened the gap between the generated information and the derived knowledge. We aim to implement a framework based on the geometric and electronic structural fingerprint of the materials. The framework will query the existing databases using the concept of similarity and map the connectivity of the materials space. As an implementation, we create a predictive model for the metal trihalide (MAX3) materials as an aim to find the predicted values of the piezoelectric constant using different regression methods like, Linear, Support Vector, Decision Tree and Random Forest.			2024

Mahaan R	The Journal of Physical Chemistry A	Sulfur Oxidation State and Substituents Influenced Multifunctional Organic Luminophores in BTP Core for OLEDs: A Computational Study on RTP, TADF Emitter and Sensitizer	The exploration of triplet excitons in thermally activated delayed fluorescence (TADF) and room-temperature phosphorescence (RTP) molecules has become a subject of significant attention and interest in recent studies. This study employed density functional theory (DFT) and time-dependent DFT theoretical methods to delve into the intricate relationship between the molecular structure and properties of molecules designed with the oxidation of sulfur atoms (S, SO, and SO2) in benzothiazinophenothiazine (BTP) core units. The calculations revealed that as the oxidation state of the sulfur atom increased, the BTP derivatives exhibited elevated ionization potentials (IPs), electron affinities (EAs), and triplet energies (ET), accompanied by reduced reorganization energies (λ), singlet energies (ES), and a S1–T1 energy gap (ΔEST). Additionally, the decrease in the exchange energy prompts a shift in the excited-state properties of molecules, transitioning them from hybridized local and charge transfer (HLCT) to charge transfer (CT) in the S1 state while maintaining their HLCT character in the T1 state. The sulfur oxidation process systematically decreases spin–orbit coupling magnitudes in the S1–T1 and T1–S0 pathways while increasing the KRISC rate, signifying a reduced propensity for phosphorescence radiative decay in oxidized molecules. Thorough investigations have explored the screening effect and orbital mixing of lone pair electrons in sulfur atoms, satisfying the desired criteria for a multifunctional RTP, TADF emitter and sensitizer.	2.9	https://pubs.acs.org/doi/full/10.1021/acs.jpca.3c05259	2023
Mahaan R	ChemPhotoChem	Converting Conventional Host to TADF Sensitizer and Hot-Exciton Emitter in Donor-Adamantane-Acceptor Triads for Blue OLEDs: A Computational Study	Exploiting triplet excitons in TADF sensitizers and hot-exciton emitters has attracted considerable attention and interest in recent studies on the design and development of blue OLEDs. The structural and optical property relationship of adamantane (Ad) core appended with four different strengths of donor and seven acceptor units were investigated using DFT and TD-DFT methods. The theoretical studies revealed that increased donor and acceptor strength on adamantane building block leads to: (i) a decrease in ionization potentials and an increase in electron affinities, (ii) a decrease in singlet energies (ES) and the S1-T1 energy gaps (ΔEST); (iii) decreased SOC magnitudes between S1-T1 states; (iv) increased RISC rate from the Tn to S1 states, demonstrating an increased tendency for upconversion of triplet excitons from the Tn to S1 state. In addition, low exchange energy causes excited state characteristics of molecules to shift from HLCT to CT nature in the S1 state. In contrast, the T1 states retain their LE character, resulting in higher triplet energies (ET). The adamantane molecular systems appended with P-DMAC-Donor-Ad-P-DMB and Donor-Ad-P-BODIPY based triads exhibit promising TADF sensitizer and hot-exciton characteristics to find application as potential candidates for blue OLEDs when compared to experimentally reported conventional host.	3.7	https://chemistry-europe.onlinelibrary.wiley.com/doi/10.1002/cptc.202300211	2023

Betsy, K. B., Mehta*, S. K., Ananthavel, A., Kakkanattu, S. P., Purushotham, P., Seetha, C. J., & Peediakal, M. P	Atmospheric Pollution Research	Role of tropical cyclones with varying intensities in the redistibution of aerosols	The study analyzes three tropical cyclones (TC) with varying intensities, namely BOB02, a deep depression in the Bay of Bengal; Tauktae, an extremely severe cyclone in the Arabian Sea (AS); and Amphan, a supercyclone in the Bay of Bengal, which developed on October 11, 2020, May 13, 2021, and May 16, 2020, respectively. The analysis focuses on studying the re-distribution of the aerosols over the Indian region using these distinct datasets: Modern-Era Retrospective Analysis for Research and Application, version 2 (MERRA2), Integrated Multi-Satellite Retrievals for GPM (IMERG), and Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observation (CALIPSO). Throughout the cyclonic period, which includes the period from the inception of the lowpressure area to its dissipation as well as the pre-cyclonic and post-cyclonic periods (one week prior to and after the cyclonic period, respectively), various parameters related to aerosols and background meteorological conditions were collected. The primary parameter of interest was the aerosol optical depth (AOD). The analysis revealed significant variations in meteorological parameters such as wind speed, temperature, relative humidity, and rainfall along the cyclone track during both the cyclonic and post-cyclonic conditions compared to the precyclonic conditions of these TCs. The AOD surrounding the cyclone track decreases during cyclonic and postcyclonic conditions compared to pre-cyclonic conditions. This is due to the scavenging of both anthropogenic and natural (dust) aerosols. Conversely, AOD increases along the cyclone track, mainly due to an increase in natural (sea salt) aerosols. During pre-cyclonic conditions, both natural (dust) and anthropogenic (black carbon, organic carbon, and sulfate) aerosols contribute significantly to the total AOD, whereas during pre-cyclonic	4.83	https://doi.org/10.1016/j.apr.2023.101990	2023

Seetha C. J, Sanjay Kumar Mehta*, Sachin Philip Kakinada, Pooja Purushotham, K. B. Betsy and Musaid P.P	Theoretical and Applied Climatology	Characteristics of the atmospheric boundary layer during transient monsoon conditions	Knowledge of atmospheric boundary layer height (ABL) during transient monsoon conditions is essential to understand the role of the monsoon on the exchange between ABL and the free troposphere (FT). The role of the Indian summer monsoon on the day-to-day variations of the ABL height over the five selected stations distributed across the northern (New Delhi), central (Nagpur), western (Mumbai), eastern (Kolkata), and southern peninsular (Gadanki) India has been investigated. In this study, radiosonde datasets over 2004–2019 are utilized to obtain the ABL height during the active and break phases of the monsoon. The India Meteorological Department (IMD) gridded rainfall dataset identifies the active and break phases based on the central India rainfall. We have observed the contrasting wind range of spatial variation in the meteorological features during the active and break monsoon conditions over these stations. Within the ABL, the temperature becomes lower and relative humidity (RH) higher during the active than the break phase over different stations across India. The inland stations show pronounced active and break differences compared to the coastal stations. All the stations have a larger active and break difference in surface meteorological parameters during the daytime compared to nighttime. The particulate matter (PM) 2.5 concentration is higher during the break phase when compared to the active phase. The active and break difference in the ABL height strongly depends on the time and space scales besides the meteorological factors. On a day-to-day scale, the relationship between the ABL and active and break phases is not straightforward, as their relationship is nonlinear. The relationship between the ABL height and active and break monsoon phases is stronger for the central inland stations than the coastal stations. Over southern peninsular India, ABL height is more related to wet and dry conditions based on the local rainfall than the central India monsoon rainfall. The ABL height becomes shallower (0.6–0.8 km) over central India	3.375	https://doi.org/10.1007/s00704-023-04578-y		2023

Kakkanattu, Sachin Philip, Mehta*, S. K. and D, Balasubrahamanyam and Rakesh, V. and Kesarkar, Amit P.,	Atmospheric Research	Thermodynamic Structure of the Atmospheric Boundary Layer Over a Coastal Station in India for Contrasting Sky Conditions During Different Seasons.	The thermodynamic structure of the atmospheric boundary layer for contrasting sky conditions over Chennai, a coastal station in the Indian subcontinent, is investigated through conserved variable analysis of equivalent potential temperature and specific humidity. Simultaneous radiosonde and micropulse lidar measurements undertaken in 2018 constitute the primary database in this investigation. One of the most prominent features of this analysis is a consistent occurrence of a double mixed layer structure during the clear-sky and cloudy conditions throughout the year. The occurrence frequency of the double mixing lines is higher during the pre-monsoon season compared with the winter and northeast (NE) monsoon seasons. The advection mainly dominates the formation of double mixing lines during the winter and pre-monsoon seasons. In contrast, convection and advection dominate during the southwest (SW) and NE monsoon seasons. The frequent double mixing lines over Chennai occur mainly from the restratification of the convective boundary layer (CBL) due to the sea-breeze onset and the cloud layer. Occasionally, a triple mixing line structure is also observed during the fair-weather boundary layer (FWBL) of the pre-monsoon and SW monsoon seasons. Among the 355 total observations collected during 2018, the first, second, and third mixing lines occurred 100%, 70%, and 14%, respectively. The thermal internal boundary layer (TIBL), CBL, and FWBL occur 50%, 97%, and 30%, respectively. The first mixing line is represented by both the TIBL and CBL, and CBL and FWBL represent the second mixing line, whereas the third mixing line is represented solely by the FWBL. The first and second mixing line shows strong seasonal variations with lower altitudes during the pre-monsoon season and higher altitudes in the SW monsoon season, almost in the same phase as the CBL variation but in the opposite phase of the TIBL variations. The CBL height attains a minimum during the winter season and maximum during the SW monsoon season, while TIBL becomes minimum during the pre-monsoon and SW monsoon seasons and maximum during winter and NE monsoon seasons	5.5	https://doi.org/10.1016/j.atmosres.2023.106915	2023
Mehta*, S. K., Ananthavel, A., V. Velu, T. Prabhakaran, G. Pandithurai and D. N. Rao	Science of The Total Environment,	Characteristics of elevated aerosol layer over the Indian east coast, Kattankulathur (12.82oN, 80.04oE): A northeast monsoon region,	The elevated aerosol layer (EAL) plays a vital role in weather and climate by modifying the Earth's radiation budget. In the present study, the EAL occurrence and its characteristics in the pre-monsoon season using micropulse lidar (MPL) observations during 2016–2018 and Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observation (CALIPSO) during 2007–2018 over Kattankulathur is being reported. We have collected 147 days (101 cases) of MPL (CALIPSO) observations during clear sky conditions in the pre-monsoon 2016–2018 (2007–2018), out of which EAL is observed for 56 days (61 cases). The EAL width is generally found to be ~2.0 km and occurs between ~1.0 km and 5.0 km. Three different types of EALs are categorized based on their altitudinal occurrence using the zero-crossing method. The EALs with their base at ~1.0–1.5 km, ~1.5–2.0 km, and ~ 2.0–3.0 km are taken as types I, II, and III, which occur for 9, 20, and 27 days, respectively. The EAL significantly modifies the total columnar aerosol optical depth (AOD). It is found that AOD, in total, within ABL and EAL, are ~0.72 (0.61), 0.28 (0.25), and 0.45 (0.36) using MPL (CALIPSO), respectively. The aerosols within ABL contribute ~38 % (41 %) while EAL ~ 62 % (59 %) to the total AOD obtained using MPL (CALIPSO). We observed that the ABL and EAL are characterized by different aerosol subtypes, such as dust marine (31 %) and smoke (~ 27 %) aerosols. Other aerosol subtypes, such as dust and polluted dust, commonly occur within the ABL (54 %) and EAL (52 %).	10.75	https://doi.org/10.1016/j.scitotenv.2023.163917	2023

Mehta*, S. K., Ananthavel, A., Reddy, T. R., Ali, S., Mehta, S. B., Kakkanattu, S. P., ... & Betsy, K. B	Pure and Applied Geophysics,	Indirect Response of the Temperature, Humidity, and Rainfall on the Spread of COVID-19 over the Indian Monsoon Region	This article examines the role of the meteorological variable in the spread of the ongoing pandemic coronavirus disease 2019 (COVID-19) across India. COVID-19 has created an unprecedented situation for public health and brought the world to a standstill. COVID-19 had caused more than 1,523,242 deaths out of 66,183,029 confirmed cases worldwide till the first week of December 2020. We have examined the surface temperature, relative humidity, and rainfall over five cities: Delhi, Mumbai, Kolkata, Bengaluru, and Chennai, which were severely affected by COVID-19. It is found that the prevailing southwest (SW) monsoon during the pandemic has acted as a natural sanitizer in limiting the spread of the virus. The mean rainfall is * 20–40 mm over the selected cities, resulting in an average decrease in COVID cases by * 18–26% for the next 3 days after the rainfall. The day-to-day variations of the meteorological parameters and COVID-19 cases clearly demonstrate that both surface temperature and relative humidity play a vital role in the indirect transport of the virus. Our analysis reveals that most COVID-19 cases fall within the surface temperature range from 24 to 30 C and relative humidity range from 50% to 80%. At a given temperature, COVID-19 cases show a large dependency on the relative humidity; therefore, the coastal environments were more prone to infections. Wavelet transforms coherence analysis of the daily COVID-19 cases with temperature and relative humidity reveals a significant coherence within 8 days.	2.335	https://doi.org/10.1007/s00024-022-03205-7	2023
Kakkanattu, S. P., Mehta*, S. K., Purushotham, P., Betsy, K. B., Seetha, C. J., & Musaid, P. P.,Sachin K Philip	Meteorology and Atmospheric Physics	Continuous monitoring of the atmospheric boundary layer (ABL) height from micro pulse lidar over a tropical coastal station, Kattankulathur (12.82° N, 80.04° E)	The continuous monitoring of the atmospheric boundary layer (ABL) height and its diurnal variation over the coastal station is generally a challenging task due to the frequent occurrence of the thermal internal boundary layer (TIBL), neutral boundary layer, and boundary layer with a strong residual layer (RL). The wavelet covariance transform (WCT) method provides robust estimates of the ABL height; however, it fails for the cases with strong RL and TIBL. Therefore, an improved fuzzy logic algorithm has been developed incorporating the sea breeze membership function besides the six membership functions used in previous studies. Fuzzy logic classifies the signals according to the membership functions based on the quality score of the individual extracted features, making it a robust method for identifying the different types of ABL. In this study, 78 days of micropulse lidar (MPL) observations over Kattankulathur (12.82° N, 80.04°E) during 2018 are utilized to identify the diurnal variation of the ABL using a fuzzy logic algorithm. Out of 78 cases, we have observed 12 convective or unstable ABL cases, 10 neutral ABL, 24 convective cases with strong RL, and 32 convective cases dominated by TIBL. For the unstable ABL, both fuzzy logic and WCT detect a similar diurnal pattern. For the neutral ABL, the stable boundary layer (SBL) does not evolve, and hence again, both fuzzy logic and WCT detect a similar ABL pattern. However, for the strong RL and TIBL cases, the ABL height obtained using the WCT method overestimates the fuzzy logic algorithm. The ABL height for various diurnal patterns obtained using fuzzy logic algorithm compares well with radiosonde observations at 05:30 IST and 17:30 IST. The daytime mean ABL height obtained using fuzzy logic compares well with the Indian monsoon data assimilation and analysis (IMDAA) re-analysis product (generated for the Indian monsoon region); however, IMDAA underestimates the night-time mean ABL height	2.065	https://doi.org/10.1007/s00703-022-00938-x	2023

Ali, S., Mehta*, S.K., Ananthavel, A., and Reddy, T. V. R.	Atmospheric Chemistry and Physics	Temporal and vertical distributions of the occurrence of the cirrus clouds over the coastal station in the Indian monsoon region	Knowledge of the spatiotemporal coverage of cirrus clouds is vital in quantifying the radiation budget of the Earth–atmosphere system. In this paper, we present the diurnal and vertical distributions of the occurrence of cirrus clouds during different seasons as well as the interannual variation in the occurrence of cirrus over Kattankulathur (12.82?N, 80.04?E) on the west coast of the Bay of Bengal. Long-term (2016–2018) continuous micropulse lidar (MPL) observations demonstrate laminar and descending cirrus clouds that occur either as single or multiple layers. The single-layer cirrus occurrence shows a diurnal pattern with frequent occurrence in the late evening (?30 %–40 %), whereas multilayer cirrus clouds occur in the early morning (?10 %–20 %). For the diurnal pattern in single-layer cirrus cloud occurrences, convective processes dominate during the premonsoon, southwest (SW) monsoon, and northeast (NE) monsoon seasons, while the freeze-drying process is favorable during the winter season. However, both convective and freeze-drying processes are dominant in the diurnal pattern of the multilayer cirrus occurrences. The occurrence reaches a maximum (?40 %) during the SW and NE monsoon seasons, and it shows a minimum (?25 %) during the winter season. The vertical distributions indicate that the maximum occurrence is confined within the tropical tropopause layer (TTL) during all seasons. Cirrus cloud rarely occurs above the tropopause; however, it frequently occurs below the TTL during all seasons. The vertical extent of the occurrence has a broader altitudinal coverage (?8–17 km) during December–March and June–September, while the altitudinal coverage is narrower during April–May (?10–17 km) and October–November (?9–15 km). Cirrus cloud occurrence also exhibits interannual variations, with higher occurrence	6.3	https://doi.org/10.5194/acp-22-8321-2022	2022

Annamalai, V & Mehta*, S. K	Climate Dynamics	Extreme Variability of the Tropical Tropopause over the Indian Monsoon Region.	The extreme variability of the tropical tropopause may serve as an important factor in understanding the critical conditions of dynamical and radiative coupling between the troposphere and stratosphere. The extreme variability of the cold point tropopause (CPT) temperature (TCPT) and height (HCPT) are examined over a tropical station, Gadanki (13.45° N, 79.2° E), using high-resolution radiosonde data during 2006–2014. We identified the extremely cold, warm, high, and low tropopauses. The extremely cold (warm) tropopause is defined as the TCPT lesser (greater) than the lower (upper) limit of the two standard deviations of its climatological monthly mean. While the extremely high (low) tropopause is defined as the HCPT greater (lesser) than the upper (lower) limit of the two standard deviations of its climatological monthly mean. In total, 161 cases comprising extremely cold (52), warm (30), high (57), and low (22) are observed. The extremely cold (187.2 ± 1.60 K, 17.3 ± 0.52 km), warm (194.2 ± 1.78 K, 16.9 ± 0.89 km), high (191.7 ± 1.78 K, 18.2 ± 0.55 km), and low (191.8 ± 2.11 K, 16.2 ± 0.38 km) tropopauses occur without preference of season. However, these extreme tropopause cases occur independently and show distinct thermal structures. The thermal structures of the extremely cold tropopause cases are often sharper, whereas the extremely warm, high, and low tropopause cases are broader. Water vapor and ozone concentrations are found to be high for the extremely warm tropopause and low for the extremely cold tropopause. Under the shallow convection, extreme temperature profiles, in general, show prominent warming between 8 and 14 km while anomalous cooling (warming) just below (above) the CPT. Plausible mechanisms responsible for extreme tropopause variabilities such as deep convection, equatorial wave propagation, transports of water vapor and ozone, and potential vorticity intrusions are examined	4.705	https://doi.org/10.1007/s00382-022-06264-7	2022

Reddy, T. R., Mehta*, S. K., Ananthavel, A., Ali, S. & Rao, D. N.	Theoretical and Applied Climatology,	Evolution of the planetary boundary layer and its simulation over a tropical coastal station Kattankulathur (12.83º N, 80.04º E)	Continuous monitoring of the planetary boundary layer (PBL) height was carried out using simultaneous observations of the micro-pulse lidar (MPL) at Kattankulathur (12.83°N, 80.04°E) and radiosonde and surface meteorological observations at Meenambakkam (13.0°N, 80.18°E) during different seasons in the year 2016 over Chennai, in the Indian east coast region. These observations provide excellent data to evaluate the performance of the five different PBL parameterization schemes from the Weather Research and Forecasting (WRF) model simulation of PBL characteristics over the coastal environment. The simulation experiments were run using Asymmetrical Convective Model version 2 (ACM2), Yonsei University (YSU), Mellor-Yamada-Janjić (MYJ), Mellor-Yamada Nakanishi and Nino level 2.5 (MYNN2), and Bougeault–Lacarrere (BouLac) schemes. The first two schemes are the first-order closure schemes, while the last three schemes are the turbulent kinetic energy (TKE) closure schemes. We have conducted the experiments for dry and wet surface conditions on clear sky days during different seasons. Under the dry surface conditions, the comparison of the simulated PBL height with observation reveals that all the schemes perform well during the daytime. However, during night-time, all the schemes except MYNN2 underestimate the observation. MYNN2 simulates the similar PBL diurnal pattern as detected by MPL. The potential temperature and relative humidity (RH) profiles from radiosonde observations at 00Z and 12Z and their surface observations at every 1-h interval from automatic weather station are also compared with simulated results. In the case of surface parameters, the WRF model underestimates the surface temperature by ~ 2 K and surface relative humidity by ~ 10–20% for the dry surface condition. However, under the wet surface condition, simulated PBL height and surface temperature (RH) overestimate (underestimate) the observation first 8 h after the rainfall		3.375	https://doi.org/10.1007/s00704-021-03770-2	2021

Aravindhavel, A., Mehta*, S. K., Ali, S., Reddy, T. R., Annamalai, V., & Rao, D. N	Atmospheric Pollution Research	Micro Pulse Lidar measurements in coincidence with CALIPSO overpasses: Comparison of tropospheric aerosols over Kattankulathur (12.82 oN, 80.04 oE)	In this paper, we present validation of the cloud aerosol lidar with orthogonal polarization (CALIOP) level 1 and level 2 tropospheric aerosols products in coincidence to Micro Pulse Lidar (MPL) observations under different sky conditions and different seasons during March 2016–December 2018 over a tropical coastal station Kattankulathur (12.83oN, 80.04oE). In total, 33 simultaneous profiles during clear-sky (18 cases) and cloudy (15 cases; 7 mid-tropospheric (MT) clouds and 8 cirrus clouds cases) conditions are observed, out of which 5, 13, 6, and 9 cases are during winter, pre-monsoon, southwest (SW) monsoon and northeast (NE) monsoon seasons, respectively. CALIOP underestimates MPL within the boundary layer and overestimates in the free troposphere during both the clear-sky and cirrus conditions. In the clear-sky conditions, the mean bias of the level 1 aerosol products is found to be 14 ± 29% (18 ± 19%) below 3.0 km (over 3–10 km) while it is 39 ± 26% (33 ± 24%) below 3.0 km (over 3–8 km) underlying the cirrus clouds. The comparison underlying the thick MT clouds is not reliable. However, a better comparison is observed in the cases of thin MT clouds. A strong seasonal variation in the vertical distribution of the aerosol loadings near the surface with maximum (minimum) loading ~0.01 ± 0.005 km 1sr 1 (~0.004 ± 0.002 km 1sr 1) is observed during the winter (SW monsoon) season. The mean bias of level 2 aerosol profiles over the altitude 0.3–5 km is found to be 14 ± 28%, 15 ± 44%, 14 ± 25%, and 24 ± 34% during the winter, pre-monsoon, SW monsoon, and NE monsoon seasons, respectively	4.83	https://doi.org/10.1016/j.apr.2021.101082	2021

Ananthavel, A., Mehta*, S. K., Reddy, T. R., Ali, S., & Rao, D. N	Atmospheric Environment	Vertical distributions and columnar properties of the aerosols during different seasons over Kattankulathur (12.82 oN, 80.04 oE): A semi-urban tropical coastal station	Seasonal characteristics of the aerosols over Kattankulathur (12.83° N, 80.04° E) is studied using Micro Pulse Lidar observations during 2016–2018 and Cloud Aerosol Lidar and Infrared Pathfinder Satellite Observation, Moderate Resolution Imaging Spectroradiometer and Ozone Monitoring Instrument datasets during 2006–2018. The vertical distribution of the aerosols is characterized as the steep decrease with altitude nearly exponentially up to 2–3 km during the northeast (NE) monsoon and winter seasons mainly dominated by clear marine and polluted continental aerosols. While it gradually decreases with altitude up to 4–5 km during pre-monsoon and southwest monsoon (SW) seasons mainly dominated by dust aerosols. The mean aerosol loadings near the surface are ~0.38 km⍰ 1 during NE monsoon and winter, ~0.30 km⍰ 1 pre-monsoon, and 0.22 km⍰ 1 during SW monsoon seasons. Such difference in the seasonal distribution of aerosol loading is mainly attributed to the difference in surface insolation, convection, long-range transport, and the atmospheric boundary layer (ABL) structure and dynamics. The ABL contributes 61%, 46%, 38%, and 63% of the overall aerosol optical depth (AOD) during the winter, pre-monsoon, SW monsoon, and NE monsoon seasons, respectively. The AOD shows a substantial seasonal variation with two local maxima during May and October and minima during January and July. The maximum and minimum AOD is found to be ~0.59 ± 0.16 and 0.4 ± 0.05, respectively. The Angstrom exponent (AE) (fine mode fraction (FMF)) shows a marked seasonal variation with a maximum value of 0.84 (0.60), indicating the dominance of finer particles during winter and minimum value of 0.54 (0.27), indicating dominance coarse particles during SW monsoon. The AE and UV aerosol index values suggest that Kattankulathur is	4.798	https://doi.org/10.1016/j.atmosenv.2021.118457		2021

Seetha C J	Theoratical and applied Climatology	Characteristics of the atmospheric boundary layer during transient conditions of the Indian summer monsoon	Knowledge of atmospheric boundary layer height (ABL) during transient monsoon conditions is essential to understand the role of the monsoon on the exchange between ABL and the free troposphere (FT). The role of the Indian summer monsoon on the day-to-day variations of the ABL height over the five selected stations distributed across the northern (New Delhi), central (Nagpur), western (Mumbai), eastern (Kolkata), and southern peninsular (Gadanki) India has been investigated. In this study, radiosonde datasets over 2004–2019 are utilized to obtain the ABL height during the active and break phases of the monsoon. The India Meteorological Department (IMD) gridded rainfall dataset identifies the active and break phases based on the central India rainfall. We have observed the contrasting wind range of spatial variation in the meteorological features during the active and break monsoon conditions over these stations. Within the ABL, the temperature becomes lower and relative humidity (RH) higher during the active than the break phase over different stations across India. The inland stations show pronounced active and break differences compared to the coastal stations. All the stations have a larger active and break difference in surface meteorological parameters during the daytime compared to nighttime. The particulate matter (PM) 2.5 concentration is higher during the break phase when compared to the active phase. The active and break difference in the ABL height strongly depends on the time and space scales besides the meteorological factors. On a day-to-day scale, the relationship between the ABL and active and break phases is not straightforward, as their relationship is nonlinear. The relationship between the ABL height and active and break monsoon phases is stronger for the central inland stations than the coastal stations. Over southern peninsular India, ABL height is more related to wet and dry conditions based on the local rainfall than the central India monsoon rainfall. The ABL height becomes shallower (0.6–0.8 km) over central India and east and west coastal regions in north India, while deeper ABL (~ 1.0–1.8 km) over northwestern India and peninsular inland regions during the active phase and vice versa during the break phase.	3.4	https://link.springer.com/article/10.1007/s00704-023-04578-y	2023
Betsy K B	Atmospheric Pollution Resea	Roles of tropical cyclones	The study analyzes three tropical cyclones (TC) with varying intensities, namely BOB02, a dee	4.83	https://doi.org	2023

Pooja Purushotham	Pure and Applied Geophysics	Characteristics of the tropical tropopause over the northeast monsoon region	Knowledge of the tracer characteristics, such as water vapor and ozone in the tropical tropopause layer (TTL), is vital in quantifying the radiation budget and critical to understanding the exchange processes between the troposphere and the stratosphere. In this study, we have characterized the tropical tropopause parameters such as the cold point tropopause (CPT) height (CPT-H) and temperature (CPT-T), convective tropopause (COT) height (COT-H) and temperature (COT-T), and the tropical tropopause layer (TTL) using radiosonde observations during 2014-2019 over Chennai (13.0oN, 80.06oE) located in the northeast (NE) monsoon region. The water vapor and ozone data from the microwave limb sounder (MLS) simultaneous to the radiosonde observations are also utilized to understand their roles on the CPT variations for different convective conditions obtained from Infrared brightness temperature (IRBT) data. CPT over Chennai becomes higher (17.6±0.3 km) and colder (189.7±0.9 K) during the winter season and lower (16.6±0.2 km) and warmer (192.1±1.0 K) during the summer monsoon season, however, not in the same month. The water vapor (CPT-W) and ozone (CPT-O) mixing ratios at CPT are found to be lower (~70±1.4 ppmv and 3.1±0.4 ppmv) during the winter season and higher (153±4.2 ppbv and 4.8±0.6 ppmv) during summer monsoon season. COT, however, becomes lower (12.4±0.3 km) and higher (13.3±0.3 km) during pre-monsoon and summer monsoon seasons, respectively. The TTL thickness is lesser (3.5±0.6 km) and greater (4.8±0.8 km) during winter and summer monsoon seasons. Over Chennai, the seasonal variation of the upper troposphere and lower stratospheric temperature, water vapor, and ozone anomalies are in phase. We have categorized tropical convections as non-penetrative and penetrative. It is observed that the TTL temperature warms with the increasing strength of the non-penetrative convections and cools for the penetrative convection.	2.07			
Pooja Purushotham	International Journal of Climatology	Thermal characteristics of the extreme tropopauses over the tropics	Extreme variability in atmospheric variables, such as rainfall, drought, heat stress, and tropical cyclones, has emerged as a conspicuous manifestation of ongoing climate change (IPCC, 2018). However, our understanding of extreme variability in the upper troposphere and lower stratosphere (UTLS), where crucial exchange processes occur, remains limited. The main focus of this study is to characterize the extreme tropopause such as extremely cold, warm, high and low due to the changes in thermal, dynamical and chemical process in the troposphere and the stratosphere. However, these extreme tropopause cases occur independently and show distinct thermal structures. The thermal structures of the extremely cold tropopause cases are often sharper, whereas the extremely warm, high, and low tropopause cases are broader. Under the shallow convection, extreme temperature profiles, in general, show prominent warming between 8 and 14 km while anomalous cooling (warming) just below (above) the CPT. In this study we have quantified Extreme Tropopause Variability over the tropics and identified underlying the drivers and mechanisms behind extreme tropopause variability. This study has also focused on the exploring the connections between extreme tropopause variability and weather and climate extremes which can provide insights into the potential amplification or modulation of extreme events.	4.14			
S. Gayathri Devi	International Conference on Nanoscience and Nanotechnology (ICONN 2021)	Ab Initio Study of Electronic Properties of Zigzag and Armchair Graphene Nanoribbon doped with B,N, and P		Poster			2021

S. Gayathri Devi	Virtual International Conference on Hierarchically Structured Materials - 2021	Effect of Doping on Structure and Electronic properties on AGNR - A DFT Study		Oral		2021
S. Gayathri Devi	ECS Journal of Solid state science and technology	Ab initio study on electronic properties of zigzag graphene nanoribbon doped with B,N, and P	https://iopscience.iop.org/article/10.1149/2162-8777/ac2326	2.2	https://www.scopus.com/inward/record.url?eid=2-s2.0-85115985497&partnerID=40&md5=6685680da6f3175cc47698232f429d08	2021
S. Gayathri Devi	International Conference On Advanced Materials And Mechanical Characterization (ICAMMC-2021)	First Principle Study on Armchair Graphene Nanoribbon doped with B,N, and P Using Density Functional Theory		Poster		2021
S. Gayathri Devi	AIU-Anveshan: Student Research Convention 2023	Graphene Nanoribbon		Poster		2023
S. Gayathri Devi	7 International Conference on Nanoscience and Nanotechnology	Effect of doping in Zigzag and Armchair Graphene Nanoribbon using Density Functional Theory		Poster		2023
S. Gayathri Devi	Surfaces and Interfaces	Doping-induced bandgap tuning in armchair graphene nanoribbons and its impact on electron transport properties on ZAPn- A DFT study	https://www.sciencedirect.com/science/article/abs/pii/S2468023023007708	6.2	https://www.sciencedirect.com/science/article/abs/pii/S2468023023007708	2023
S. Gayathri Devi	International Conference on Thin Films and Nanotechnology-Knowledge, Leadership and Commercialization	Electron Transport studies of Zigzag Graphene Nanoribbon Doped with B,N, and P using Density Functional Theory		Poster		2023
Gayathri J K	molecules	Effect of Chalcogenophenes on Chiroptical Activity of Twisted Tetracenes: Computational Analysis, Synthesis and Crystal Structure Thereof	synthesis of peri-substituted tetracenes from their tetrahaloderivatives using Pd(0)-catalyzed C-C cross-coupling and study of chiroptical activity computationally	4.6	https://doi.org/10.3390/molecules28135074	2023

Dr. Anjan Bedi	y:proceedingsmaterials today:	Synthesis of 4,4′-Dibutyl-5,5′-di(thiophen-3-yl)-2,2′-bithiazole for applications toward organic electronic materialNovel Series of Diaminoanthraquinone-Based π-Extendable Building Blocks with Tunable Optoelectronic Properties	new bithiazole-based small molecule was synthesized and characterized by 1H NMR, 13C NMR, and HRMS and computational analysis of photophysical propetiesa new series of DAAQ based building block n-TIPS-DAAQs were syntheiszed and its tunable optoelectronic properties were studied.	3.2	https://doi.org/10.1016/j.matpr.2021.07.438	2022
Ganesh M	ACS omega Thieme(Organic Materials)	Cyclopenta[c]thiophene- and Diketopyrrolopyrrole-Based Red-Green-Blue Electrochromic Polymers	we report the first solution-processable red homopolymer (P1) of a thiophene-capped derivative of CPT (DHTCPT), and a blue homopolymer (P2) of N-substituted thienodiketopyrrolopyrrole (DEHTDPP). Additionally, by alternatingly copolymerizing the DHTCPT and DEHTDPP units, we achieved the green copolymerP3, thus completing the red-green-blue color wheels.	4.1	https://doi.org/10.1021/acsomega.2c03609	2022
Evangeline David	MDPI(Polymers)	Origin of Optoelectronic Contradictions in 3,4-Cycloalkyl[c]-chalcogenophenes: A Computational StudyCircularly Polarized luminescence(CPL) from solution and aggregation in benzotriazole based small molecules and polymers	we compare a series of 3,4-cycloalkylchalcogenophenes by tuning them atomistically using group-16 elements. Additionally, the effect of systematically extending these building blocks in the form of oligomers and polymers is studied. The size of the 3,4-substitution affected the morphology ofthe oligomers.	6	https://doi.org/10.3390/polym15214240	2023