SPRING 2025 ACS MEETING

Division of Physical Chemistry POSTER SESSION

Prof. Francesco Paesani, *Organizer*

San Diego Convention Center

Hall B2/C

Tuesday, March 25 | 7:00pm – 9:00pm

We gratefully acknowledge the support of our generous sponsor!

The Journal of Chemical Physics

Chemical Physics Reviews

Poster Board # 759: Detailing mechanistic formation of SAPO-5 using different phosphorus sources templated by new pyridinium organic template, *Presented by Jehad Al Issa*.

Poster Board # 760: Self-healing ability of perovskites under dynamic equilibrium explored by single-particle spectroscopy, *Presented by Aito Takeuchi*.

Poster Board # 761: Probing radical reactions on the surface of interstellar ices, *Presented by Carina Hobbs*.

Poster Board # 762: Cloud condensation nuclei activity of fresh and aged phenolic acid aerosol particles, *Presented by Emily Nortmann*.

Poster Board # 763: Predicting H_2O+ H_2 collision rate coefficients for rotational state-to-state transitions using mixed quantum/classical theory (MQCT), *Presented by Carolin Anna Joy*.

Poster Board # 764: Tunneling Dynamics within Classical Mechanics: An Eikonal Equation based approach, *Presented by Bijoy Dey*.

Poster Board # 765: Neuromorphic computing with energy efficient quantum materials, *Presented by Nika Bondar*.

Poster Board # 766: Using computational chemistry to elucidate the structure-function relationship and kinetics of carbon monoxide-releasing molecules, *Presented by Zahra Linsky*.

Poster Board # 767: Machine-learning assisted grand canonical sampling framework for nuclear quantum effects in constant potential electrochemistry, *Presented by Shenzhen Xu*.

Poster Board # 768: Understanding the physicochemical behavior of microplastics in lipid model membranes, *Presented by Haley Betterton*.

Poster Board # 770: Thermodynamics studies of L-threonine in aqueous1-butyl-3-methylimidazolium chloride solutions over the temperature range T = (288.15-318.15) K, *Presented by Tarnveer Kaur*.

Poster Board # 771: Anomalous fluorescence quenching in fluorous solvent-added media, *Presented by Deepika Gahlawat*.

Poster Board # 772: Aggregation in deep eutectic solvents (DESs): Formation of polar DES-in-nonpolar DES microemulsions, *Presented by Anushis Patra*.

Poster Board # 773: Ultrafast lattice dynamics in 2D hybrid perovskites enabled by strong-field THz pulse, *Presented by Zi-Jie Liu*.

Poster Board # 774: Elucidating photoswitching mechanism for super-resolution fluorescence microscopy, *Presented by Gaeun Go*.

Poster Board # 775: Development of 3D nanoimaging of semiconductor nanopatterns via super-resolution fluorescence microscopy, *Presented by Uidon Jeong*.

Poster Board # 776: Many-body effects determine the propensity of halides for the air-water interface, *Presented by Henry Agnew*.

Poster Board # 815: Hot electron chemistry on bimetallic titanium nitride core-shell nanoparticles, *Presented by Stephanie Hoang*.

Poster Board # 815: Hot electron chemistry on bimetallic titanium nitride core-shell nanoparticles, *Presented by D'Angelo Alvarez*.

Poster Board # 816: Mapping the solvation landscape: Advanced sampling and unsupervised learning to unveil free energy and structure correlations in liquid systems, *Presented by Xiaoxu Ruan*.

Poster Board # 817: Protein folding mechanisms from graph driven search, *Presented by Ziad Fakhoury*.

Poster Board # 818: Theory and quantum dynamics simulations of exciton-polariton motional narrowing, *Presented by Wenxiang Ying*.

Poster Board # 819: Non-destructive steady-state and time-resolved photoluminescence characterization of photovoltaic devices, *Presented by Christian Oelsner*.

Poster Board # 820: Non-Linear tuning of hydrophobicity by changing the composition of ternary mixtures, *Presented by Elio Casalini*.

Poster Board # 821: Encapsulation of Sb_2S_3 and Sb_2Se_3 within carbon and boron nitride nanotubes, *Presented by Griffin Milligan*.

Poster Board # 822: Response of energetic materials under focusing shock waves, *Presented by Senpeng Lin*.

Poster Board # 823: Energetic processing of sulfur-containing icy dust grains in the interstellar medium, *Presented by Elsa Yuan*.

Poster Board # 824: Humidity driven spontaneous OH radical-initiated oxidation of pure organic aerosols, *Presented by Christian George*.

Poster Board # 825: Accurate modeling of aqueous phase chemistry with rigorous physical principles, *Presented by Suman Saha*.

Poster Board # 826: Direct Quantification of Van der Waals forces in layered graphene structures: formalism development and insights from single and multifrequency AFM, *Presented by Chia-Yun Lai*.

Poster Board # 826: Direct Quantification of Van der Waals forces in layered graphene structures: formalism development and insights from single and multifrequency AFM, *Presented by Matteo Chiesa*.

Poster Board # 827: Network methods for characterizing emergent structures in multi-body interactions, *Presented by Elizabeth Diessner*.

Poster Board # 828: Dimer charge-transfer complex junctions enabled by silver electrodes, *Presented by Yihao ZHANG*.

Poster Board # 829: Nonlinear semiclassical spectroscopy of ultrafast molecular polariton dynamics, *Presented by Michael Reitz*.

Poster Board # 830: Continuous flow fabrication of homogeneous covalent organic framework thin films for enhanced QCM-based adsorption kinetic studies, *Presented by Wen-Yi Yu*.

Poster Board # 831: Zundel-like complex formed between anions in sulfuric acid aqueous solutions, *Presented by Sijia Chen*.

Poster Board # 832: Kinetics of methane clathrate substitution by liquid ethane under Titan-relevant conditions, *Presented by Tuan Vu*.

Poster Board # 883: Thermodynamics phases of HIV-1 capsid self-assembly using coarse-grained molecular dynamics simulations, *Presented by Casey Hsu*.

Poster Board # 884: Development of a theoretical approach to constrain the abundance of pyrene in TMC-1, *Presented by Thomas Speak*.

Poster Board # 885: Extension of the Canongia Lopes-Padua ionic liquid force field to thiazolium cations, *Presented by Adam Sturlaugson*.

Poster Board # 886: Synthesis and electrochemical study of chlorophenyl thiophene, *Presented by Spencer Berger*.

Poster Board # 887: Protein-based adsorbents for uremic toxin clearance in chronic kidney disease patients, *Presented by Henrike Wagler*.

Poster Board # 888: Establish protein containers as building blocks for the assembly of anisotropic nanorods into optical hybrid materials, *Presented by varnika yadav*.

Poster Board # 889: Exploring water dynamics on the alumina surface using neural network potentials and enhanced sampling techniques, *Presented by Venkata Surya Kumar Choutipalli*.

Poster Board # 890: Metal disulphide Fe/Co/Ni as superior electrocatalyst for overall water splitting, *Presented by Urvashi Gondaliya*.

Poster Board # 891: Tailored air-aqueous interface with self-assembled oligomers for enhanced direct air capture of CO_2: A molecular dynamics perspective, *Presented by Nitesh Kumar*.

Poster Board # 892: Electrochemistry of methylphenyl thiophene, *Presented by Max Gawlik*.

Poster Board # 893: Nitrate photolysis in solution from first principles molecular dynamics and machine learning, *Presented by Kam-Tung Chan*.

Poster Board # 894: Spin dynamics simulations of multi-metal center Molecular qudits, *Presented by Noah Huerta*.

Poster Board # 895: Data-driven many-body framework for organic molecules, *Presented by Alison Rhoads*.

Poster Board # 896: Efficient peripheral coarse-graining simulation method for accelerating large-scale biomolecular processes, *Presented by Akarsh Kumar Dash*.

Poster Board # 897: Operating a multi-level molecular dimer switch through precise tip-molecule control, *Presented by Yueqing Shi*.

Poster Board # 898: Optimization of core-shell bimetallic nanoparticles for enhanced photocatalytic reactions, *Presented by Melia Hernandez*.

Poster Board # 898: Optimization of core-shell bimetallic nanoparticles for enhanced photocatalytic reactions, *Presented by Aidan Tran*.

Poster Board # 900: Computational studies of the anion effect on water permeability of DOPC membranes in the presence and absence of cholesterol, *Presented by Rodney Versace*.

Poster Board # 901: Probing the nature of hydrogen bonding networks at interfaces using SERS, *Presented by Archishman Sarkar*.

Poster Board # 902: Solid-state high harmonic generation in common large bandgap substrate materials, *Presented by Ezra Korican-Barlay*.

Poster Board # 903: Two-Photon absorption of BODIPY, BIDIPY, GADIPY, and SBDIPY, *Presented by Ismael Elayan*.

Poster Board # 904: Excited state anti-aromaticity relief as a quantitative descriptor of photobasicity, *Presented by Marco Hernandez*.

Poster Board # 905: Determining adsorption of volatile organic compounds on single-crystalline ice utilizing sum frequency generation (SFG) spectroscopy, *Presented by Luca Manning*.

Poster Board # 906: Time-dependent wettability evolution of graphite surfaces: The dominant role of water adsorption revealed by experimental and quantum simulations, *Presented by Chia-Yun Lai*.

Poster Board # 907: Synthesis and Characterisation of Bismuth Selenide for degradation and kinetic studies of anionic dyes under thermal and photochemical conditions, *Presented by Umesh Utkoor*.

Poster Board # 908: Toward data-driven many-body simulations of biomolecules with chemical accuracy, *Presented by Zoe Solomon*.

Poster Board # 909: *In-situ* synthesized Cu-doped α-Fe_2O_3 (hematite) nanorods and its application in photoelectrochemical water splitting for green hydrogen production, *Presented by Ans Bin Tariq*.

Poster Board # 910: General overview of Single Walled Carbon Nanotubes as optical nanosensors, *Presented by Gabriel Núñez*.

Poster Board # 911: Impacts of halide salts on the decomposition kinetics of aqueous carbonic acid, *Presented by Daniel Esterman*.

Poster Board # 952: Developing an instrument for kinetic measurements of reactions involving interstellar aromatic molecules, *Presented by Reace Willis*.

Poster Board # 953: Joint computational and experimental study of the reactions between $N(^2D)$ and simple aromatic hydrocarbons, *Presented by Marzio Rosi*.

Poster Board # 954: Photochemistry of aqueous reduced sulfur species under anoxic conditions, *Presented by Jackson Witkow*.

Poster Board # 955: Light-driven CO_2 release directly from naphtholates, *Presented by Berk Delibas*.

Poster Board # 956: Kinetic studies of the disproportionation of aqueous sulfite under anoxic conditions, *Presented by Raider Horn*.

Poster Board # 957: Simulating chemical dynamics on a parametrically driven bosonic quantum device, *Presented by Pouya Khazaei*.

Poster Board # 959: Photoelectric driven metalation of tetraphenyl porphyrin on copper nanowire coated electrodes, *Presented by Zhanxian Gong*.

Poster Board # 960: *In-situ* adsorption analysis of drug guest molecules in covalent organic frameworks (COFs) via quartz crystal microbalance with dissipation (QCM-D), *Presented by Pei-Chen Huang*.

Poster Board # 962: Probing the electrode-electrolyte interface in copper electrodeposition: Insights from first-principles calculations, *Presented by Sergio Correal*.

Poster Board # 963: Atomic-scale simulations to uncover the molecular mechanisms of HIV capsid protein maturation, *Presented by Caroline Cannistra*.

Poster Board # 964: High-capacity reversible hydrogen storage in bihenylene monolayer decorated with NLi_4 superalkali cluster: Insights from first-principles simulations, *Presented by Preeti Beniwal*.

Poster Board # 965: Infrared spectral analysis of extraterrestrial ices observed by JWST, *Presented by Andrew Turner*.

Poster Board # 966: Adenine formation in a prebiotic scenario, *Presented by Stefano Ferrero*.

Poster Board # 967: Utilizing ultrafast time-resolved vibrational sum frequency generation spectroscopy to probe photoinduced reactions on surfaces, *Presented by Erykah Foss*.

Poster Board # 968: Stabilizing Ru-formyl CO_2 reduction intermediates by formation of Lewis acid adducts, *Presented by James Shipp*.

Poster Board # 969: Shedding light on the surface composition of aqueous aerosols, *Presented by Samantha Perri*.

Poster Board # 970: Investigating the effects of microplastics on calcitonin structure and aggregation, *Presented by Olivia Tancredi*.

Poster Board # 971: Electronic structure of the 3d metal series of mono acetylide cations, *Presented by Haritha Kolavathra Sasi*.

Poster Board # 972: Growth and characterization of layered multimolecular architectures on monolayer MoS_2, *Presented by Anoushka Ghosh*.

Poster Board # 973: Hot electron chemistry on bimetallic gold core-shell nanoparticles, *Presented by olivia guyette*.

Poster Board # 973: Hot electron chemistry on bimetallic gold core-shell nanoparticles, *Presented by Brianna Zamora*.

Poster Board # 974: Electronic spectrum of gas-phase niobium hydride, NbH, *Presented by Thomas Varberg*.

Poster Board # 975: Computational investigation of antibacterial drug candidates based on a 1,2, 4 oxadiazole linker, *Presented by Roberto Nunez*.

Poster Board # 976: Hidden optical nonlinearities in linear polaritonic spectra, *Presented by Arghadip Koner*.

Poster Board # 978: Investigating local environment effects of intramolecular proton transfer dynamics in anthrarufin, *Presented by Yingshi Feng*.

Poster Board # 979: Computational modeling of DNA-based aptamers targeting EGFRvIII+ receptors in glioma, *Presented by Gaurav Sharma*.

Poster Board # 980: Using biphenyl to probe the effect that annealing has on the surface morphology of vapor deposited chloroalkanes on Al_2O_3, *Presented by Jesse Nieman*.

Poster Board # 981: Femtosecond X-ray solution scattering illuminates membrane protein dynamics, *Presented by C. Swathi K. Menon*.

Poster Board # 982: Synthesis and characterizations of graphene-based quantum dots synthesis for biological imaging, *Presented by Hoang Long Nguyen*.

Poster Board # 983: Interfacial water structure at the charged graphene/water interface using vibrational sum-frequency generation spectroscopy, *Presented by Toheeb Balogun*.

Poster Board # 984: Perfect lattice match does not necessitate the maximum heterogeneous ice nucleation, *Presented by Wanyu Zhao*.

Poster Board # 985: Electrochemical evaluation of 1,3,4-thiadiazole derived moieties for mild steel in varied pH environments, *Presented by Sheetal Sheetal*.

Poster Board # 987: Supramolecular design and assembly engineering toward high performance organic field-effect transistors, *Presented by Mingliang Li*.

Poster Board # 988: Time-resolved spectroscopy of optically active tethered bisarylmethanes, *Presented by Camille Schubert*.

Poster Board # 1011: Potential energy surfaces (PESs) and mechanism of the reactions of cyclopentadiene with methylidyne and ethynyl: A theoretical study, *Presented by Sabrina Arias*.

Poster Board # 1012: Study of photophysical properties of ethidium bromide and its application in determining water dynamics in hydrated NafionÂ® film, *Presented by Phuong Ho*.

Poster Board # 1013: Comparison of plasmonic enhanced photoluminescence of upconversion nanoparticles, *Presented by Caroline Friedersdorf*.

Poster Board # 1014: Infrared spectroscopy of ethanium cations in helium nanodroplets, *Presented by Marc Moroz*.

Poster Board # 1015: Electrochemistry of Nitro thiophene, *Presented by Adisyn O'Connor*.

Poster Board # 1016: Photostable single-photon emission from atomically precise $Au_{24}(SCH2Ph\text{-}^{t}Bu)_{20}$ nanoclusters for quantum computing applications, *Presented by Abhrojyoti Mazumder*.

Poster Board # 1017: Controlling the rate of hydrolysis at the air-water interface, *Presented by Kenneth Judd*.

Poster Board # 1018: Data-driven model for predicting dehydrogenation barriers in magnesium hydride: Accelerating solid-state hydrogen storage design, *Presented by Xiujing Xing*.

Poster Board # 1019: Design strategies for solvent-mediated effective interaction between silica nanoparticles in water, *Presented by Yuvraj Singh*.

Poster Board # 1020: High-performance near-infrared OLEDs maximized at 925 nm and 1022 nm through interfacial energy transfer, *Presented by Chieh-Ming Hung*.

Poster Board # 1021: Microemulsion-based synthesis of highly efficient $AgNO_3$-doped fibrous silica-titania (FST) photoanodes for PEC Water Splitting, *Presented by samia arain*.

Poster Board # 1022: Biochemical activity and photocatalytic dye degradation in the Ag doped Fe2O3/NiO2 nanocomposite, *Presented by musfira arain*.

Poster Board # 1023: Size-tunable MoS_2 quantum dots for enhanced solar cell applications, *Presented by Dominick Hernandez*.

Poster Board # 1024: Shining a light on antimicrobial peptide pore formation: Effects of charge distribution on Alamethicin pore structure, *Presented by Rhys Edwards*.

Poster Board # 1025: Development of non-adiabatic ring polymer molecular dynamics for strong light-matter interactions, *Presented by Ziying Cao*.

Poster Board # 1026: Light-induced open-circuit potential in Noble and oxide-forming metals in electrolytes, *Presented by Noemi Salazar*.

Poster Board # 1027: Simulating electronic charge transfer rates in complex molecular systems, *Presented by Zongwei Huang*.

Poster Board # 1028: Plasmon driven electron transfer, *Presented by Elizabeth Rehwinkel*.

Poster Board # 1029: Modulating the reactivity of an antenna-reactor Al@TiO_2 plasmonic photocatalyst by modifying annealing conditions, *Presented by Aliyu Ahmad*.

Poster Board # 1030: Novel liquid nano-sheet sample delivery in femtosecond X-ray scattering, *Presented by C. Swathi K. Menon*.

Poster Board # 1031: Evaluation of aliphatic alcohols for CO_2 capture using the characteristic carbonate frequency, *Presented by Keerthy P. Sudhakaran*.

Poster Board # 1032: Dissecting the fluorescence quenching pathways of aminocoumarins in solution through ultrafast spectroscopy, *Presented by Jiawei Liu*.

Poster Board # 1033: Redox conduction through cytochrome 'nanowires' can sustain cellular respiration, *Presented by Matthew Guberman-Pfeffer*.

Poster Board # 1035: Retinal mobility in visual rhodopsin explored using electronic structure calculations, *Presented by Lauren Thaller*.

Poster Board # 1036: Unconventional Off-to-On switch in Excited-State Intramolecular Proton Transfer with derivatives exhibiting light-induced proton-coupled charge transfer for directional counterion translocation, *Presented by Kai-Hsin Chang*.

Poster Board # 1037: Tuning the proton dynamics of merocyanine-based photoacids with alcohols, *Presented by Sebastian Perez Munoz*.

Poster Board # 1038: Synthesis, Characterization and Electrocatalytic evaluation of cobalt phosphides in water splitting, *Presented by Wajiha Fatima*.

Poster Board # 1039: Role of solar photolysis in the atmospheric removal of methacrolein oxide and the methacrolein oxide-water van-der Waals complex in pristine environments, *Presented by Lily Guidry*.

Poster Board # 1040: Exploring optical asymmetry in the N-doped chiral carbon dot and their application in fluorescence off-on sensing of Hg2+ and L-Cys, *Presented by ANGANA BHATTACHARYA*.

Poster Board # 1041: Leveraging cross peak-specific two-dimensional electronic spectroscopy to reveal coherences contributing to energy transfer in C-Phycocyanin 620, *Presented by Keerthi Vaasan Mani*.

Poster Board # 1042: Kinetic analysis of dye adsorption on DNA: Effect of ionic strength, *Presented by Srijana Pandey*.

Poster Board # 1043: Gas phase rovibrational and electronic spectroscopy of magnesium-containing molecules relevant to astrochemistry, *Presented by Nathan Deyonker*.

Poster Board # 1044: Ultrafast photochemistry of 4-nitrophenol at the air-water interface, *Presented by Aziz Mohammed*.

Poster Board # 1067: Time-resolved photoluminescence measures charge transfer chains from heterobinuclear units to electron shuttles, *Presented by Charlotte Caracansi Bizup*.

Poster Board # 1068: Wrinkle-accompanied phase transition between α and β' In2Se3, *Presented by Lina Kodaimati*.

Poster Board # 1069: Exploring transformations in elemental sulfur using a machine-learned interatomic potential, *Presented by Sonia Salomoni*.

Poster Board # 1070: First principles simulations of optical rotation of chiral molecular crystals, *Presented by Emmanuel Forson*.

Poster Board # 1071: Spectroscopic insights into zinc porphyrin: Elucidating the effect of structural heterogeneity on excited-state dynamics in solution and solid phase H-aggregates, *Presented by Emma Orcutt*.

Poster Board # 1072: Translator Assembly for pulsed supersonic expansions, *Presented by Channing Christian*.

Poster Board # 1073: Compressive sensing in sum frequency generation microscopy, *Presented by Sarah Ortiz*.

Poster Board # 1075: Comprehensive analysis of trimethoprim binding with cyclodextrins in aqueous solutions: Experimental and computational insights, *Presented by Sonika arti*.

Poster Board # 1076: Nitrocellulose model for molecular dynamics simulation and its interactions with nitroglycerin, *Presented by Timothy Schutt*.

Poster Board # 1077: Coarse-grained simulations of HIV maturation within viral particles, *Presented by Sinai Lee*.

Poster Board # 1078: Lanthanide-doped MoS_2 monolayers for single-photon emitters: Density functional theory study of defect formation and electronic properties, *Presented by Hyosik Kang*.

Poster Board # 1079: Exploring the relative contributions of scattering and interference signals in interferometric scattering (iSCAT) spectroscopy of plasmonic nanoparticles, *Presented by Sanjay Sridhar*.

Poster Board # 1080: Understanding molybdenum disulfide monolayer reactivity with zinc oxide nanobubbles: A theoretical study, *Presented by Christian A. Celaya*.

Poster Board # 1081: Investigating molecular structure in beta-hairpin proteins using cyano-substituted tryptophan probes and 2D IR spectroscopy, *Presented by Majid Hassani*.

Poster Board # 1082: Effects of Dipyridinium thiazolo[5,4-d]thiazole on the charge transport properties of organic electronics, *Presented by Ryan Kolaitis*.

Poster Board # 1083: Vibrational polariton infrared spectral simulations based on cavity quantum electrodynamical density functional theory within Gaussian atomic basis, *Presented by Zheng Pei*.

Poster Board # 1084: Computational prediction of tip enhanced Raman spectroscopy of Mercaptopyridine under reductive and oxidative electrochemical conditions, *Presented by Lindsey Madison*.

Poster Board # 1085: Esterification via aerosolization: A green chemistry approach, *Presented by Justin Wang*.

Poster Board # 1086: Towards all-optical determination of nanoparticle size, structure, and composition using CLocK microscopy, *Presented by Zachary O'Dell*.

Poster Board # 1087: Coiled-coil peptides: A template for investigating relationship between stability and sequences using fluorescence auto-quenching, *Presented by Mandy Blackburn*.

Poster Board # 1088: Predicting water clustering patterns around succinimide, *Presented by Yuki Watanabe*.

Poster Board # 1089: Modelling of NMR spectra in proteins: Hartree-Fock approximations, density functional theory and neural network corrections, *Presented by Emilio Ramirez Contreras*.

Poster Board # 1090: Interfacial chemistry of sub-micron-sized droplets using nonlinear light scattering, *Presented by Saranya Pullanchery*.

Poster Board # 1091: QTAIM, bond order and surface analysis of $NgBNH^+$ (Ng=Ar-Rn), *Presented by Fatma Selampinar*.

Poster Board # 1092: Unraveling the mechanisms of peptide hydrogel assembly through molecular dynamics simulations of peptide pairs in water system, *Presented by Xinyue He*.

Poster Board # 1093: Fluorescence detection of photogenerated hydroxyl radicals in synthetic melanin, *Presented by Ruby Mitchell*.

Poster Board # 1094: Orientation distribution of crystalline β-sheet domain in *B.*moro silk fiber studied with vibrational sum frequency generation (SFG) spectroscopy, *Presented by Jihyeong Ryu*.

Poster Board # 1095: Determination of cellular uptake of anti-body nanoparticles by yeast cells, *Presented by Aaron Cerda*.

Poster Board # 1096: Examination of photoluminescence in rhodamine 6G, *Presented by David Graupner*.

Poster Board # 1097: Computational studies of the environmental photochemical degradation of emerging contaminants in marine relevant ecosystems, *Presented by Londyn Bardash*.

Poster Board # 1098: Silanol functionalization of amorphous silica surface, *Presented by Shreyaa Brahmachari*.

Poster Board # 1099: Elucidating water's underlying local structures through geometric analysis, *Presented by Hua Yuan*.

Poster Board # 1100: Synthesis of $Mo_xW_{1-x}S_2$ by hydrothermal synthetic methods for pollutant degradation, *Presented by Francisco Contreras*.

Poster Board # 1123: Hydrogel composition effects on performance as single-walled carbon nanotube purification media, *Presented by Kevin Tvrdy*.

Poster Board # 1124: Long molecular wires and the auto-ionization of water, *Presented by Yezhi Jin*.

Poster Board # 1125: Time-resolved measurements of electron transfer from heterobinuclear units through electron shuttles to silica defects, *Presented by Adam Hill*.

Poster Board # 1126: Time-scale analysis of neutrino detection in organic scintillator using a high quantum efficiency photomultiplier tube, *Presented by David Shelden*.

Poster Board # 1127: Kinetic study of pseudo-first and second-order degradation of Methyl Green under basic conditions, *Presented by Marco Allard*.

Poster Board # 1128: Role of borohydride ligand in depicting the covalency in actinide complexes, *Presented by Nathan Loutsch*.

Poster Board # 1129: Exploring physical properties of trehalose-derived deep eutectic solvents with acetylcholine chloride and betaine, *Presented by Jenna Lipani*.

Poster Board # 1130: Effect of additives on the thermal conductivity of polypropylene: a molecular dynamics study, *Presented by Kelsey Stocker*.

Poster Board # 1131: Investigating the effects of charge distribution on membrane-active antimicrobial peptides through the development of single-vesicle dye leakage studies, *Presented by Claire Stoddard*.

Poster Board # 1132: Phase transitions of manganese dioxide structural polymorphs, *Presented by galilee samuels*.

Poster Board # 1133: Development of parallel Crystal algorithm towards photochemical reaction discovery in molecular photoswitches, *Presented by ankit pandey*.

Poster Board # 1134: Discovering phenomena in the atmospheric removal of isoprene-derived organic hydroperoxides, *Presented by Layla Pongracz*.

Poster Board # 1135: Tetraarylphosphonium-based task-specific ionic liquids with exceptional thermal stability, *Presented by Muhammadiqboli Musozoda*.

Poster Board # 1136: Piezoresponse in WO_3 thin films: Towards energy harvesting, *Presented by Manuel Ramos*.

Poster Board # 1137: Developing a chemically accurate data-driven many-body model for triplet oxygen hydration, from the gas to condensed phase, *Presented by Omkaar Kulkarni*.

Poster Board # 1137: Developing a chemically accurate data-driven many-body model for triplet oxygen hydration, from the gas to condensed phase, *Presented by Shreya Gupta*.

Poster Board # 1138: Biophoton interactions with tau protein, *Presented by Carter Brand*.

Poster Board # 1139: Ring puckering dynamics in cyclopentanone derivatives, *Presented by Tatiana Cardoso*.

Poster Board # 1140: Leveraging ab initio molecular dynamics for force field development at electrochemical interfaces, *Presented by Andrew Vizzard*.

Poster Board # 1141: Decomposition and oxidation of methanol on platinum (111), *Presented by Min Gi Kang*.

Poster Board # 1142: Modeling Glyme mixtures for sodium-ion electrolytes: impacts of anion identity and Glyme mixing at electrode surfaces, *Presented by Eileen Park*.

Poster Board # 1145: Extensive characterization of carbon dot nanostructures synthesized from Phenylenediame polymerization pathway, *Presented by Joel Asare*.

Poster Board # 1147: Modification of silk fibroin using plasma-enhanced chemical vapor deposition with small and large molecules, *Presented by Mollie Corbett*.

Poster Board # 1147: Modification of silk fibroin using plasma-enhanced chemical vapor deposition with small and large molecules, *Presented by Bethany Yashkus*.

Poster Board # 1148: Molecular mechanisms of chromophore release from cellular-retinaldehyde binding protein (CRALBP) in the visual cycle, *Presented by Daniel Santos*.

Poster Board # 1149: Thermodynamic consistency and fluctuations in mesoscopic stochastic simulations of reactive gas mixtures, *Presented by Changho Kim*.

Poster Board # 1150: Heavy atom-free photoredox catalysis: Mechanistic insights into π-extended BODIPY dye-based catalysts, *Presented by Charlotte Fuqua*.

Poster Board # 1151: Single-molecule infrared spectroscopy on Cu(100) with scanning tunneling microscopy, *Presented by Kangkai Liang*.

Poster Board # 1152: High-Q cavities reveal quantum vacuum effects in linear response, *Presented by Sricharan Raghavan Chitra*.

Poster Board # 1153: Simulation of macroscopic hydrogel formation using monte carlo methodologies, *Presented by Christopher Salazar*.

Poster Board # 1154: Science Explorer (SciX) - a NASA-funded multidisciplinary digital library, *Presented by Olivia Wilkins*.

Poster Board # 1155: Investigations into the DNA-binding mode of doxorubicinone, *Presented by Samantha Glazier*.

Poster Board # 1156: Multi-wavelength study of comet C/2022 E3 (ZTF)-complementary ALMA and JWST investigations of H_2O and CH_3OH in cometary comae, *Presented by Kiernan Foster*.

Poster Board # 1191: Theory of resonant suppression in vibrational polariton chemistry, *Presented by Pengfei Huo*.

Poster Board # 1192: Constructing effective multi-state Hamiltonian for charge transfer in organic photovoltaic systems, *Presented by Xiang Sun*.

Poster Board # 1193: Visualizing back electron transfer in photoredox catalysis by single molecule imaging, *Presented by Chunming Liu*.

Poster Board # 1194: Artificial neural networks and high-throughput synthetic approaches for building a chemical space predictor model of perovskite materials, *Presented by Md. Ataur Rahman*.

Poster Board # 1195: Lighting up magnetic resonance: The role of the exchange interaction in optically polarized organic chromophore-radicals, *Presented by Claudia Avalos*.

Poster Board # 1196: Universality and variability of dynamic emission Stokes shift in lead halide perovskites, *Presented by BO ZHANG*.

Poster Board # 1197: Investigating the optimal properties of $ZnSnO_x$ through annealing treatment with real-time resistivity monitoring, *Presented by Aitkazy Kaisha*.

Poster Board # 1198: Ehrenfest modeling of vacuum fluctuations under strong light-matter coupling, *Presented by Ming-Hsiu Hsieh*.

Poster Board # 1199: Bright state distribution anomaly in excitonic molecular tubes: Accessing short wavelength information with optical spectroscopy, *Presented by Chern Chuang*.

Poster Board # 1200: Investigating the effect of aligned nanorods as a medium for luminescent solar concentrator devices: a detailed analysis using ergodic Markov chains, *Presented by Jonathan McTague*.

Poster Board # 1201: Microscopic reversibility is a critical consideration when performing Stern-Volmer quenching analysis of excited-state proton transfer of strong photoacids, *Presented by SHIRLEY CHANG*.

Poster Board # 1202: Carrier-induced dynamics in ferroelectrics probed by femtosecond stimulated Raman spectroscopy, *Presented by Man Tou Wong*.

Poster Board # 1203: Exploring exciton lifetime in STM break junction under the applied fields, *Presented by Yuchen Wang*.

Poster Board # 1204: Linear and nonlinear optical response based on many-body Bethe-Salpeter and Kadanoff-Baym approaches for two-dimensional Janus semiconductors, *Presented by Dmitry Skachkov*.

Poster Board # 1205: H-bond dynamics modulated by vibrational polaritons: Inhomogeneous broadening matters, *Presented by Tianlin Liu*.

Poster Board # 1206: Cavity mediated ultrafast chemical exchange under vibrational strong coupling, *Presented by Haochuan Mao*.

Poster Board # 1207: Ultrafast Formation of Charge Transfer Trions at Molecular-Functionalized 2D MoS_2 Interfaces, *Presented by Ethan Jing*.

Poster Board # 1208: Quantification of titanium and other elements in mineral ilmenite collected from Neelam Valley employing calibration free laser induced breakdown (CF-LIBS) spectroscopy and energy dispersive X-ray spectroscopy (EDX), *Presented by Altaf Ahmad*.

Poster Board # 1209: Light-molecule interactions including conical intersections using a simplified configuration interaction-corrected Tamm-Dancoff approach, *Presented by Lei Xu*.

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Poster Board # 1220: Effects of oxygen vacancies on charge carrier dynamics and photocatalytic efficiency of cerium oxide nanoparticles, *Presented by Bach Pham*.

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Poster Board # 1261: Probing vibronic interaction driven electron dynamics by 2DIR spectroscopy, *Presented by Ranadeb Ball*.

Poster Board # 1262: Cyanamide vibrational probes as an investigative tool on hydration shell dynamics and viscosity using 2D IR spectroscopy, *Presented by Christopher Mallon*.

Poster Board # 1263: DFT-based calculation of vibrational sum frequency generation spectral features of crystalline Î²-sheets in silk: polarization and azimuth angle dependences, *Presented by Jihyeong Ryu*.

Poster Board # 1264: Excitons and optical properties of ZnO ferritin nanoparticles by photoluminescence (PL) spectroscopy, *Presented by Delwar Hossain*.

Poster Board # 1266: Excited-state absorption coefficients of porphyrin derivatives via direct deconvolution of transient absorption spectra, *Presented by Lampros Tzianos*.

Poster Board # 1267: Characterizing ultrafast vibrational dynamics of Lehn's catalyst on porous silicon with transmissive and reflective 2DIR, *Presented by Rebecca Hopkins*.

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Poster Board # 1272: Heterogeneous astrocatalysis of space-abundant transition metals, *Presented by Gerard Pareras*.

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Poster Board # 1277: Possible formation of corundum in the circumstellar medium, *Presented by Rebecca Firth*.

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Poster Board # 1282: Fuel-driven self-assembly of transient naphthalene diimide cages with tunable pathway-dependent optoelectronic properties, *Presented by Jarek Maleszka*.

Poster Board # 1283: Investigating resonant near-field heat transfer through thermal emission measurement of molecules under vibrational strong coupling, *Presented by Ju Eun Yim*.

Poster Board # 1284: Engineering zinc Porphyrin-based superstructures for covalent stapling in organic solvents, *Presented by Ifigeneia Tsironi*.

Poster Board # 1285: Formation and growth of dust grains in our Universe, *Presented by Gunnar Nyman*.

Poster Board # 1287: Formation and spectral analysis of larger aluminum nitride clusters, *Presented by Charles Palmer*.

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