

SPRING 2026 ACS MEETING

Division of Physical Chemistry POSTER SESSION

Prof. Bern Kohler, *Organizer*

Georgia World Congress Center

B3/B4 Exhibit Hall

Wednesday, March 25 | 6:00pm – 8:00pm

We gratefully acknowledge the support of our generous sponsor!

**The Journal of
Chemical Physics**
Chemical Physics Reviews

Poster Board 11: Tunable photochemical properties of silica gel Belousov-Zhabotinsky micro-reactors: Synthesis and temperature characterization. Presented by Kudakwashe Shumba

Poster Board 12: Efficient four-component density functional theory. Presented by Jonathan Bersson

Poster Board 13: Time-dependent density functional theory benchmarks for astrobiology calculations: Chlorophyll and other putative extraterrestrial photopigments. Presented by Roberto Peverati

Poster Board 14: Role of ligands in SERS performance of gold nanoparticles. Presented by Emma Riseborough

Poster Board 15: Envisioning quantum mechanical DFT models validated by infrared spectroscopy. Presented by Robert Allsopp

Poster Board 16: Emergent magnetism in two-dimensional xf ($x = \text{Ca}, \text{Sr}, \text{Ba}$) electrenes. Presented by Dmitry Novoselov

Poster Board 17: Use of a closed-shell reference to compute rovibronic spectral data for open-shell molecules with EOM-CC. Presented by Rebecca Firth

Poster Board 18: Asymmetric stability: The hidden driver of directional protein secretion. Presented by Lan Yang

Poster Board 20: *In-operando* spectroscopy reveals charge transfer mechanisms on TiO_2 photocatalyst. Presented by Jakob Liggons

Poster Board 21: Probing the distribution of water's self-ions at diverse aqueous interfaces: Implications for nanobubble stability and interfacial reactivity. Presented by Pengchao Zhang

Poster Board 22: Tuning vibrational coupling strength between hyperbolic media and organic molecules. Presented by Courtney Ragle

Poster Board 23: Capillary molecular combining of DNA with 3D printed tools for use in genome optical mapping. Presented by Dylan Smith

Poster Board 24: Unlocking the conformational secrets of DYRK1A kinase with computational microscope: Exploring phosphorylation-driven structural dynamics. Presented by KAPIL URSAL

Poster Board 25: Dubnium vs. Tantalum: Computational interpretations of directly identified heavy element molecular species for comparison with transition metal analogues. Presented by Sarah Sprouse

Poster Board 26: Ultrafast charge transfer dynamics in perylene-modified nucleic acids: Computational design principles for enhanced DNA imaging. Presented by Solomon Effah

Poster Board 27: Incorporation of photoactive polyacenes into well-defined framework materials. Presented by Yujing Wang

Poster Board 28: Quantum chemical predictions of PAH IR spectra. Presented by Nolan White

Poster Board 29: Bio-compatible metal-organic frameworks towards targeted protein interactions in cystic fibrosis. Presented by Lydia Yates

Poster Board 48: Symmetry dilemmas in quantum computing: A comprehensive analysis. Presented by Muhan Zhang

Poster Board 49: Coacervate-assisted mineral leaching for phosphorylation in a primordial soup. Presented by Sean Zsoldos

Poster Board 50: Acidity of actinide oxide-hydroxide complexes. Presented by Eddy Lontchi

Poster Board 51: Ab initio descriptions of high-symmetry polycyclic aromatic hydrocarbons and their anion resonance states. Presented by Karl Lyu

Poster Board 52: Integrating NMR constraints into molecular dynamics to refine models of vancomycin:peptidoglycan binding. Presented by Macarena Machado Combe

Poster Board 53: Taming S^2 : Symmetry-conserving quantum algorithms for electronic structure. Presented by Ilias Magoulas

Poster Board 54: Probing ultrafast symmetry breaking and bond dissociation pathways of methane cation with x-ray transient absorption spectroscopy. Presented by Kevin Marin

Poster Board 55: Quantum chemical spectral data for the astronomical detection of the potentially prebiotic 2-iminoacetaldehyde and 1,2-diiminoethane. Presented by Megan McKissick

Poster Board 56: Refractive indices for binary solutions of two n-alkanes and binary solutions of a n-alkane and a primary alcohol. Presented by William Miller

Poster Board 57: Membrane binding of alpha synuclein as reported by covalently attached thiocyanate vibrational probe groups. Presented by Perla Villegas Minyety, Yassine Falah and Abby Ryan

Poster Board 58: Hydroxyl radical generation in synthetic melanin exposed to UVA radiation. Presented by Ruby Mitchell

Poster Board 59: Sodium dodecyl sulfate (SDS) surfactant effects on lipid bilayer dynamics. Presented by Nikhil Modayur

Poster Board 60: Auramine-o and thioflavin-t as probes for reaction medium dynamics. Presented by Mallory Mohon

Poster Board 61: Influence of counterion size on the stability of doped $\ddot{\text{I}}\text{E}$ -conjugated polymers. Presented by Niharika Mullanpudi

Poster Board 62: Single molecular magnetism in sandwiched organometallic complexes. Presented by Sakshi Nain

Poster Board 63: High resolution infrared spectroscopy of radicals in helium nanodroplets. Presented by Sachin Nambiar

Poster Board 64: Salt-induced diffusiophoresis of a cationic micelle in water: Determination of cross-diffusion coefficients. Presented by Josie Nguyen

Poster Board 65: Electronic transition changes in aerosols of organic air pollutant catechol derivatives. Presented by KatieAnn Nguyen and Ashley McDonald

Poster Board 88: Molecular dynamics simulations of $\hat{\text{I}}^2$ -lactam antibiotic binding to *Staphylococcus aureus* penicillin-binding proteins. Presented by Olatunde Olademehin

Poster Board 90: Examining differences in the triplet vs. singlet excited state reactivities of bromonaphthol isomers. Presented by Esther Pak

Poster Board 91: QM/MM at solid surfaces: Negotiating long-range electrostatics and boundaries. Presented by John Pederson

Poster Board 92: Exploring methanesulfinic acid surface activity at various ionic strength and pH conditions. Presented by Erica Peterson

Poster Board 93: Growth dynamics of colloidal plasmonic nanoparticles monitored by *In situ* Second harmonic generation, extinction spectroscopy, and two-photon fluorescence. Presented by Stena Peterson

Poster Board 94: Computational exploration of the catalytic decomposition of hydroxylamine on Ir(111). Presented by Jack Poulos

Poster Board 95: Coaxial arrays for strong coupling & molecular polaritonic applications. Presented by Courtney Ragle

Poster Board 96: Formation of plastic nanotriangles and their use in single particle interaction studies. Presented by Edin Osmanbasic

Poster Board 97: Unraveling symmetry-breaking charge transfer in ALICE-MOF. Presented by Nikita Gupta

Poster Board 98: Temperature-dependent interfacial dynamics of nanoplastics in mimetic respiratory cell membranes. Presented by Zhane Norris

Poster Board 99: Kinetic theory and crystallography: RMS velocities as predictors of subsurface mineral deposits. Presented by Salako Olatunji

Poster Board 100: Microscopic rate constants and mechanistic branching in electrochemical oxidation: A qm/mm dynamics perspective. Presented by John Hymel

Poster Board 101: Mutual correlation: From strongly entangled electrons to multi-component dynamics. Presented by Francesco Evangelista

Poster Board 102: Reliable prediction of isotope fractionation factors. Presented by Amila Prasanna Rajapaksha Rajapaksha Palle gedara

Poster Board 103: Using computation to rationalize the unexpected excited state proton transfer pathways of a photobase containing a built-in hydrogen bonding group. Presented by Faith Ramirez

Poster Board 104: Distance and orientation dependence of triplet-triplet energy transfer couplings based on nonorthogonal multireference wave functions. Presented by Saptarshi Saha

Poster Board 105: Exploring lewis photobasicity in metal complexes. Presented by Cole Sanchez

Poster Board 106: Gas phase redox potentials, acidities, and heats of formation of halomethane fragmentation derivatives using G3(MP2). Presented by Cole Seely

Poster Board 161: Phototriggering for time resolved crystallography in heme enzymes. Presented by Drisha Sehgal

Poster Board 163: Formation of a silicon-carbon hybrid material from reacting silicon nanoparticles with acetylene. Presented by Chandi Sheffield

Poster Board 164: Operando Raman spectroscopy study of surface charge transfer mechanisms. Presented by Meikun Shen

Poster Board 165: Magnetic field effects on photoinduced electron transfer reactions involving thionine acetate incorporated into ionic micelles. Presented by Joseph Shuler

Poster Board 166: Synthesis and study of electrochemical properties of naphthoquinone derivatives containing antiparasitic and naphthoquinoxaline derivatives containing antitumor activities. Presented by Sajjan Silwal

Poster Board 167: Time-resolved laser photolysis and steady-state fluorimetry study of non-arrhenius behavior of pyrene excimer formation reaction. Presented by Molly Smock

Poster Board 168: Probing polymorph and chirality-dependent singlet fission dynamics in dipyrrolonaphththyridinedione (DPND) crystal via transient absorption microscopy. Presented by Karamoko Soumahoro

Poster Board 169: Probing the phase behavior of catanionic mixtures of surfactants using steady-state and time-resolved electron paramagnetic resonance. Presented by Max Spies

Poster Board 170: Investigating excited state pathways of Schiff base naphthols. Presented by Kathryn Stomma

Poster Board 171: Microfluidic system for real-time characterization from molecular to nanoscale in flow. Presented by Jiajun Tian

Poster Board 172: Using Excel's Solver and VBA to solve particle-in-a-bumpy-box problems. Presented by James Hall

Poster Board 173: Electron-stimulated desorption of trihydrogen cation, "the molecule that made the universe," from water ice. Presented by SUNny He

Poster Board 174: Trends in protonation states of alkyl organic acids across functional groups at the air-water interface. Presented by Katherine Holt

Poster Board 175: Methodological considerations in RT-TDDFT simulations of intermolecular Coulombic decay. Presented by Owen Holt-Frank

Poster Board 176: *In situ* kinetic study of pH-dependent interactions between molecular drugs and covalent organic frameworks (COFs) via quartz crystal microbalance with dissipation detection (QCM-D). Presented by Pei-Chen Huang

Poster Board 177: Aqueous loss mechanisms of reduced sulfur species in prebiotically-relevant conditions and their implications for planetary habitability. Presented by Kylee Hutchinson

Poster Board 178: Pyridine based stilbene as a photochromic switch in donor acceptor systems. Presented by Lola Ibragimova

Poster Board 179: Unraveling plasmon-mediated small-molecule activation by Silver nanoclusters using time-dependent DFT. Presented by Paul Javed

Poster Board 202: Measuring the binding affinity of the dye Pyronin y with cucurbit[n]urils using fluorescence correlation spectroscopy. Presented by Farooq Khan

Poster Board 203: Possible mechanism for enantiomeric selectivity of a luminescent chiral lanthanide complex induced by a chiral deep eutectic solvent. Presented by Valentine Klimkowski

Poster Board 204: Employing a focal point approach with higher-order corrections to compute accurate experimental binding energies of van der waals dimers. Presented by Luke Kurfman

Poster Board 205: Basis set effect on linear response density functional theory calculations on periodic systems. Presented by Emmanuel Forson

Poster Board 206: Spin delocalization in electrochemically and chemically oxidized triarylamine radical cations of donor-bridge-acceptor molecules probed by EPR spectroscopy. Presented by Charlotte Fuqua

Poster Board 207: Maximum entropy polymer model predicts the architectural effects of genetic structural variations. Presented by Miles Gantcher

Poster Board 208: Transient absorption spectroelectrochemistry of a PEDOT:PSS electrode. Presented by Caitlyn Clark

Poster Board 209: Machine learning prediction of infrared spectra for CO₂ binding to amine sorbents. Presented by Taylor Cole

Poster Board 210: Solvent-resolved A, B, C routes for the hydrogenation of carbonyls. Presented by Damian Duda

Poster Board 211: Hexamer rings of cyclo-cyclopropenyliene with carbon, oxygen, and sulfur. Presented by Charlie Earl

Poster Board 212: Modifying self-assembly parameters to control nanoparticle-metal-organic framework composite catalyst formation. Presented by Reagan Elia

Poster Board 212: Modifying self-assembly parameters to control nanoparticle-metal-organic framework composite catalyst formation. Presented by Emily Curbow

Poster Board 213: Eu²⁺-doped cspbb₃ Nanocrystals exhibiting dual emission for optoelectronic applications. Presented by Shanas Fatima

Poster Board 214: Optimization of a coarse-grained model for RNA based on parameters for DNA. Presented by Maria Fernald

Poster Board 215: Rovibrational analysis of methanetriol and its conformers. Presented by Nathaniel Carlson

Poster Board 216: Color tunability and optical thermometry study of Er³⁺ Co-doped SrMoO₄: Dy³⁺ Phosphor. Presented by Satyam Chaturvedi

Poster Board 217: Investigation on formulations of curcumin and characterizations. Presented by Changqing Chen

Poster Board 218: Mechanistic studies on the excited state dynamics of 9,10-dicyanoanthracene. Presented by Shi Fang Chen

Poster Board 219: Stabilizing CASSCF: Combining embedding and orbital projection to maintain a robust active space. Presented by Zhijian Chen

Poster Board 220: Investigating the effects of a charged residue on alamethicin's pore formation ability. Presented by Emma Cheung

Poster Board 275: *Ab Initio* modeling of photoelectron angular distributions as a probe into anionic resonances. Presented by Carlos Roberto Bean Chevez

Poster Board 276: Analyzing the electronic structure of ethylene *via* high-level correlation and orbital optimization. Presented by John Bell

Poster Board 277: Ultrafast excited state dynamics of a highly strained olefin in solution. Presented by Meseret Bezabih

Poster Board 278: Synthesis and characterization of UiO-66-NH₂ for potential low-cost explosive detection. Presented by Lauren Bigelow

Poster Board 279: Identification of amyloid proteins via machine learning enhanced 2D IR spectroscopy. Presented by Dalton Boutwell

Poster Board 280: Mechanistic study of propene metathesis on heterogeneous catalyst. Presented by Shreyaa Brahmachari

Poster Board 281: Development of a raspberry pi-based electrochemical gas sensor system with principal component analysis. Presented by Catherine Byrne

Poster Board 282: Characterization of early actinide complexes using advanced electronic structure theory methods. Presented by Kayleigh Barlow

Poster Board 283: Structural and energetic properties of Pd nanoclusters. Presented by Shane Autry

Poster Board 284: Elara: A sounding rocket based radio telescope array for measuring the neutral hydrogen spectral line. Presented by Samuel Arnold

Poster Board 285: Charge transport and relaxation dynamics in layered Ruddlesden-Popper perovskite: Sr₃Ti₂O₇. Presented by Anjali Antony

Poster Board 285: Charge transport and relaxation dynamics in layered Ruddlesden-Popper perovskite: Sr₃Ti₂O₇. Presented by Alok Shukla

Poster Board 286: Covariance-based MD simulation analysis pinpoints nanobody attraction and repulsion sites on SARS-CoV-2 omicron spike protein. Presented by Fareeda Abu-Juam

Poster Board 287: Proton pachinko: Tracking the excited-state intramolecular proton transfer of St. John's Wort-derived fluorescent photosensitizer hypericin with ultrafast spectroscopy. Presented by Seth Johnson

Poster Board 288: Investigation of ball milling for post-synthetic exchange in UiO-66. Presented by Anya Marie Dela Merced

Poster Board 289: Mitigating overestimation in rehydroxylation dating: Residual hydroxyls and the role of firing temperature in ancient pottery. Presented by Kylie McCoy

Poster Board 290: Investigating structure-function relationships for the valorization of coal combustion residuals through carbon capture. Presented by Noah Smith

Poster Board 290: Investigating structure-function relationships for the valorization of coal combustion residuals through carbon capture. Presented by Ruby Soto

Poster Board 291: Halomethane radicals, halocarbene, and halocarbyne thermochemistry at the G3(MP2) level: Reduction potentials, bond dissociation energies, and pK_a in solution. Presented by Thomas Andress

Poster Board 292: Unravelling the surface polarity landscape of $\hat{I}\pm$ -synuclein fibrils via pseudo hyperspectral fluorescence imaging. Presented by Tonima Nandy

Poster Board 316: Tunable Auxetic response of wrinkled graphene oxide Sheets: Linking wrinkle orientation and Spacing to Poisson's ratio. Presented by Oliver D'Anna

Poster Board 317: Quantifying adsorbate-adsorbate and adsorbate-substrate interactions on carbon-based substrates using the ABC isotherm. Presented by Grayson Camp

Poster Board 318: Predicting the mixed gas Reactions of SO_2 and H_2O with TiO_2 Nanoclusters : H_2SO_3 or SO_2/h_2O Chemisorption? Presented by Timeria Jackson

Poster Board 319: Chiral selectivity using ternary deep eutectic solvents. Presented by Ashton Lake

Poster Board 320: Enantioselectivity using ternary chiral deep eutectic solvents. Presented by Hayden Teague

Poster Board 321: III-V semiconductors bulk v. surface. Presented by Quinlon Williams

Poster Board 322: Functionalization of olefins through electrochemistry: A study of ionic liquid/water systems. Presented by Chloe Renfro

Poster Board 323: Investigating the spectral tuning of iLOV using computational methods. Presented by Isaac Bare

Poster Board 324: Biphasic buffer system. Presented by Mahele Tamanna

Poster Board 325: Kinetics of plcg1 mutant lysates on a suppolipid bilayer. Presented by Stephanus Yang

Poster Board 326: Modeling vitamin D activation in different cellular environments using TDDFT. Presented by Vicky Villarosa

Poster Board 327: Tuning fractal graphene properties via background gas in chamber synthesis. Presented by Shusil Sigdel

Poster Board 328: Investigation and characterization of Cocrnife/nm heterostructures and their influence on the spin Seebeck effect. Presented by Maryam Maryam

Poster Board 329: Enhancing reusability of graphene-based electrochemical sensors through defect mitigation. Presented by Alex Medeiros

Poster Board 330: Examining local electric field effects in conducting polymers using vibrational spectroelectrochemistry. Presented by Ryan Spencer

Poster Board 331: Illuminating resonant modes in STM-BJ plasmonic cavities. Presented by Oliver Tan

Poster Board 332: Spectroscopic and computational study of xylazine's vibrational and electronic states when affected by hydrogen bonding. Presented by Brandon Suh

Poster Board 333: Supported ionic liquid phase material from graphitic carbon nitride and 1,8-diazabicyclo[5.4.0]undec-7-ene based protic ionic liquid: An advanced catalytic system for photodegradation of levofloxacin from aqueous solution. Presented by GULSHAN ARA

Poster Board 334: Titanium-based materials for tritium capture in high-temperature gas-cooled reactors: Insights from density functional theory on support and promoter roles. Presented by Sung Gu Kang

Poster Board 389: Improved CCSD(T) using DFT references for transition-metal thermochemistry. Presented by Barbaro Zulueta

Poster Board 390: Machine learning-guided robotic optimization of anion exchange doping in conjugated polymers. Presented by Kevin Liebetau

Poster Board 391: Measuring the Bond dissociation energies of transition metal Cyanides/Isocyanides. Presented by Samantha Stinson

Poster Board 392: Carbodicarbenes as hydride donor catalysts in heteroallene reductions. Presented by Max Schernikau

Poster Board 393: Infrared band strengths and optical constants of D₂O ices with new measurement on H₂O ices. Presented by Yukiko Yarnall

Poster Board 394: Theoretical study of plutonium hydroxide complexes.

Presented by Elizabeth McRae

Poster Board 396: Quantifying Dexter energy transfer from extra faceted

perovskite nanocrystal to organic dyes. Presented by Mrinal Kanti Panda

Poster Board 397: Sulfate radical-driven pathways in CdS quantum dot-catalyzed

nitrobenzene reduction. Presented by Chao Wang

Poster Board 398: Predicting the mixed gas reactions of SO₃ and H₂O with TiO₂

nanoclusters: H₂SO₄ or SO₃/H₂O chemisorption?. Presented by Ashley Sanchez

Poster Board 399: Comparative study of graphene oxide reduction: Examining the influence of laser, chemical, thermal, and solar methods on material properties.

Presented by Alex Medeiros

Poster Board 400: Predicting the reactions of H₂S with TiO₂ nanoclusters:

Preliminary insights into titanium bisulfide formation. Presented by Kennedy

Green

Poster Board 401: Characterizing merocyanine-based photoacid dynamics in

alcohols for carbon capture. Presented by Juyeon Lee

Poster Board 402: Computation study of the spin trapping potential of gallic acid

towards hydroxyl free radicals. Presented by Renolph Gaglo

Poster Board 403: Computational study of noncovalent interactions at the

poloxamer-protein interface. Presented by Leann Saura

Poster Board 404: Beyond the ensemble average: Single-molecule

characterization of rhodamine fluorescence. Presented by Jake Ankrum

Poster Board 405: Harnessing 2D perovskite biexciton light sources for quantum

communication. Presented by Zijian Gan

Poster Board 406: Machine-learned atom-typed damped electrostatics and

induced point dipole models for accurate non-covalent interactions. Presented by

Austin Wallace

Poster Board 407: Mechanistic understanding of PET ester bond scission on dual-

site models: A purely theoretical study. Presented by Hengyue Xu

Poster Board 428: Switching between topological phases in double Moiré hBN-

graphene-hBN heterostructure with twist angles. Presented by Renu Sangwan

Poster Board 429: Ligand shell density controls photoinduced detachment in colloidal CdSe quantum dots. Presented by Jacob Cho

Poster Board 430: Resolving dispersive diffusion in layered perovskites with photocurrent-detected transient gratings. Presented by Saba Mahmoodpour

Poster Board 431: Assessment of the DLPNO approximation for two-body contributions to crystal lattice energies. Presented by Jaden Yon

Poster Board 432: Probing redox-state-dependent IR signatures of flavin: Computational assignment of difference-FTIR bands in solution. Presented by Ngan Le

Poster Board 433: Resolving uphill energy transfer from red chlorophylls of photosystem I-Light harvesting complex I via two-dimensional electronic spectroscopy. Presented by Cooper Costello

Poster Board 434: Tuning spin dynamics and circularly polarized light emission in chiral 0D bismuth-iodide perovskites. Presented by cheng yang

Poster Board 485: High-resolution imaging of deuterated methanol in the Orion KL Nebula. Presented by Boriana Yotzova

Poster Board 485: High-resolution imaging of deuterated methanol in the Orion KL Nebula. Presented by Olivia Wilkins

Poster Board 486: Disentangling exciton relaxation and charge transfer in polymer-gold nanoparticle hybrid systems. Presented by Megan Redding

Poster Board 487: Effect of ZnO oxygen vacancies on the photocatalytic reaction pathways. Presented by Alexander Kestner

Poster Board 488: DFT QSAR model for CDK6 inhibitors as breast cancer treatment. Presented by Grace Gottschalk

Poster Board 489: Water-in-fluorous solvent microemulsions: Media for (bio)molecular solvation. Presented by Deepika

Poster Board 516: Generating room temperature ferroelectric nematic liquid crystal mixtures for optical applications. Presented by Anna Hamilton

Poster Board 517: Visualizing 3-dimensional Schlieren imaging with anaglyphs. Presented by Shivam Patel

Poster Board 518: Investigation of solute solvation within renewable solvents *via* pyrene fluorescence. Presented by Anuj Sharma

Poster Board 519: Microsolvation effects of 1,1-dimethyl-biguanide hydrochloride (metformin). Presented by Jasmine Sanders

Poster Board 520: Ultrafast dynamics of ammonium thiocyanate under vibrational strong coupling. Presented by Avram Gutierrez

Digital Posters

Poster D1: Cdft theory based approach to predict the quenching rate of excited state carbazoles ioners in bimolecular electron transfer reactions. Presented by Meenu Meenu

Poster D3: Electrochemical and surface studies of selenium-modified gold electrodes. Presented by Lily Mansfield and Karan Philip

Poster D4: P-nitro-phenylalanine provides a new report on the inside of the *E. coli* fatty acid acyl carrier protein. Presented by Avani Marmer

Poster D5: Fundamental and applied aspects of electrochemical processes in an alkaline manganese dioxide commercial galvanic cell: An upper-level experimental physical chemistry laboratory experience. Presented by Bratoljub Milosavljevic

Poster D6: Ab initio investigation of interactions between the super oxide radical and CO₂. Presented by Wafaa Fawzy

Poster D7: Computational study of interactions between the superoxide radical and thymine. Presented by Johnnie Perry

Poster D8: Hybrid glyco-inhibitors of lectins: Multivalency vs specificity. Presented by Roya Jafari

Poster D9: Computational insights into the messy world of quantum dot surfaces. Presented by Dibyajyoti Ghosh

Poster D10: Computational determination of pKa of bio-organic carboxylic acids in aqueous medium. Presented by Triston Smith

Poster D11: Mechanistic insights into the role of outer membrane properties in β -barrel outer membrane protein folding: A molecular dynamics simulation study. Presented by Hanyao Wang

Poster D12: Surface ordering and electronic characterization of polynuclear porphyrins at the solid-liquid interface. Presented by Chiranjeevulu Kashi

Poster D13: Chemistry at Mach 5+: Plasma-informed oxidation and ablation of HfB₂ and ZrB₂. Presented by John-Ryan Lawrence

Poster D14: Raman spectroscopic study of a CrSBr intercalation compound. Presented by Bianca Fernandez

Poster D15: Probing spin-correlated radical pair evolution in donor-chiral bridge-acceptor molecules using photo-CIDNP. Presented by Ashly Gasior

Poster D16: Simultaneous search of five chiral molecules in Orion KL (OMC-1). Presented by Ana Margarita Gomez Romo

Poster D17: Do metalloproteins regulate net charge to control the energetics of electron transfer? Presented by Matthew Guberman-Pfeffer

Poster D18: Identification of pyrolysis products of 2-chloro-2-methylpentane using matrix-isolation Fourier transform IR spectroscopy. Presented by Benjamin Campbell

Poster D19: TiO₂ nanocorals and FeTiO₃ perovskite oxide for enhanced functional properties. Presented by Monerah Alosaimi

Poster D20: Effects on actin filament polymerization induced by molybdenum disulfide (MoS₂). Presented by Tristen Gerren

Poster D21: Implementing Automated hybrid QM/MM APEC-F 2.0 to investigate the tunability of flavin's one- and two-electron reduction potentials in "improved" light-oxygen-voltage (iLOV) sensing proteins. Presented by SARAH ELHAJJ

Poster D22: Raman spectroscopic and quantum chemical investigation of ethylene carbonate molecular clusters. Presented by Kenneth Arnett

Poster D23: Absolute quantum yield of IR1061 in chloroform. Presented by Conner Brower

Poster D24: Comparison of experimental and computational oxidation reaction enthalpies of fatty acids. Presented by Jaycie Massengale

Poster D25: Ultrafast spin relaxation in 2D perovskites by correlated exciton fluctuations. Presented by Shuyue Feng

Poster D26: Kinetic and product studies of Trimethyl(trifluoromethyl)silane oxidation. Presented by Ramesh Sapkota

Poster D27: Influence of ionic liquid on surfactant induced partially unfolded proteins. Presented by Rajkumar Sahoo and Mintu Halder

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