

**SPRING 2024 ACS MEETING**

**Division of  
Physical Chemistry  
POSTER SESSION**

Prof. Julie Biteen, *Organizer*

Ernest N. Morial Convention Center

Hall C

Tuesday, March 19 | 7:00pm – 9:00pm

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**The Journal of  
Chemical Physics**

**Chemical Physics Reviews**

**Poster Board #428:** Applying nanoscale infrared spectroscopy to study structural changes within A $\beta$  40 peptide. *Presented by Tanmayee Naik.*

**Poster Board #430:** Estimate of the C-Cl photoionization cross section and absolute photoionization cross sections of chlorinated organic compounds. *Presented by Yilan Chen.*

**Poster Board #434:** Molecular dynamics tools to inform intercalation of 2D spin-active materials for fine tuning quantum spin liquid state. *Presented by Timothy Schutt.*

**Poster Board #438:** Ultrafast exciton dynamics in the anthracene dimer. *Presented by Alexander Lemmens.*

**Poster Board #442:** Broadband microscopic inquiry of the excited state structure function relationship in diattenuating perylene diimide materials. *Presented by Skyler Hollinbeck.*

**Poster Board #446:** Study of the ionization potential, electron affinity, HOMO-LUMO gaps and NLO in C<sub>62</sub>O<sub>2</sub>H<sub>14</sub> molecule. *Presented by Ongun Ozcelik.*

**Poster Board #448:** Surface loading dictates triplet production via singlet fission in dye-sensitized metal oxide films. *Presented by Melissa Gish.*

**Poster Board #527:** Theoretical study of the gas phase reaction of OH radical with cyclopentenone derivatives. *Presented by Emmanuel Ubana.*

**Poster Board #531:** Observation of vibronic signatures in 2DIR of TCNQ. *Presented by Ranadeb Ball.*

**Poster Board #535:** Experimental and computational studies of gas hydrates. *Presented by Adebayo Adeleye.*

**Poster Board #539:** Reliable and simple computational method for the characterization of complex molecular systems using IR spectroscopy. *Presented by Laura Sepulveda.*

**Poster Board #543:** Ballistic energy transport via long alkyl chains: A new initiation mechanism. *Presented by Sithara Nawagamuwege.*

**Poster Board #547:** Coherent vibrational wavepacket dynamics: Advancing our understanding for the role of molecular vibrations in photochemical reactions. *Presented by Pyosang Kim.*

**Poster Board #530:** Experimental baseline for understanding the ultrafast dynamics of thiocyanate bioorthogonal probes. *Presented by Joe Shirley.*

**Poster Board #534:** Blackbody infrared radiative dissociation under vibrational strong coupling. *Presented by Enes Suyabatmaz.*

**Poster Board #538:** Vacuum ultraviolet absorption studies of subcritical and supercritical methanol. *Presented by Timothy Marin.*

**Poster Board #542:** Modeling fast electron dynamics with non-Hermitian real-time time-dependent density functional theory. *Presented by Yi-Siang Wang.*

**Poster Board #546:** Ground-state quantum-electrodynamical density functionals for strong light-matter coupling in optical cavities. *Presented by Anna Baranova.*

**Poster Board #550:** Assessing modulations of molecular properties under cavity polariton formation using angle-resolved photoluminescence excitation spectroscopy. *Presented by Elizabeth Odewale.*

**Poster Board #629:** Infrared and rotational spectral data for cyclic carbon monoxide dimers & carbon suboxide isomers. *Presented by Olivia Harwick.*

**Poster Board #633:** Characterizing hydrates inhibition by glycoproteins via molecular dynamics simulations. *Presented by Gabriel Miles.*

**Poster Board #637:** Exploring ion exchange effects on the immersion freezing efficiency of a model sodium Y zeolite. *Presented by Ryan Mitch.*

**Poster Board #643:** Molecular entanglement witness by absorption spectroscopy in polariton chemistry. *Presented by Weijun Wu.*

**Poster Board #647:** Towards a topological classification of nonadiabaticity in chemical reactions. *Presented by Christopher Daggett.*

**Poster Board #626:** Mechanism of non-Kasha fluorescence in pyrene. *Presented by Sourav Majumdar.*

**Poster Board #630:** Temperature influence on the hydration, dynamic, and dielectric properties of  $\text{AlCl}_3$  electrolytic aqueous solutions: A molecular dynamics approach. *Presented by Abdelkbir Errougui.*

**Poster Board #634:** Intermolecular interaction and ionic hydrogen bonding studies of hydroxylammonium nitrate clusters. *Presented by Shinae Kim.*

**Poster Board #638:** Ultrafast plasmon-induced hot-electron transfer process in epitaxial noble metal-semiconductor heterostructures. *Presented by Li Zhai.*

**Poster Board #642:** Investigating strong coupling between silicon quantum dots and acene triplet states. *Presented by Maryam Baraazandeh.*

**Poster Board #725:** Structure and properties of phospholipid-based microbubbles determined by steady-state electron paramagnetic resonance. *Presented by S. Ivan Weaver.*

**Poster Board #729:** Effect of lithium salt on fluorescence quenching in glycerol: A comparison with ionic liquid/deep eutectic solvent. *Presented by Manish Kumar.*

**Poster Board #733:** Mixed micelle formation by sodium dodecylsulfate and dodecyltrimethylammonium bromide in aqueous ionic liquid media. *Presented by Anjali.*

**Poster Board #737:** Challenges and solutions in pH measurements up to concentrated NaCl solutions. *Presented by Bahram Hosseini Monjezi.*

**Poster Board #741:** Formation of Al<sub>2</sub>O<sub>3</sub> and other aluminum oxides in the interstellar medium. *Presented by Rebecca Firth.*

**Poster Board #728:** Exploring the interactions between antifreeze proteins and lipid membranes. *Presented by Emily Vernon.*

**Poster Board #732:** Microwave spectra of ethanesulfonic acid and its monohydrate. *Presented by Wei Lin.*

**Poster Board #736:** Self-trapped exciton mediated energy transfer to Sm<sup>3+</sup> in Cs<sub>2</sub>Agi<sub>1-x</sub>Sm<sub>x</sub>Cl<sub>6</sub>:Bi double perovskite nanocrystals. *Presented by Rachna.*

**Poster Board #740:** DFT+F12 QFFS for cost effective rovibronic spectroscopy. *Presented by Noah Garrett.*

**Poster Board #744:** Synthesis and characterization of Na-doped Zn<sub>2</sub>GeO<sub>4</sub> optical fibers. *Presented by Emelie Cintron.*

**Poster Board #748:** Precision engineering of MOF thin films: Enabling advanced optical sensing and microelectronics. *Presented by Bahram Hosseini Monjezi.*

**Poster Board #827:** Advancing semiempirical quantum chemistry with extended Lagrangian and machine learning. *Presented by Maksim Kulichenko.*

**Poster Board #833:** Electronic spectroscopy of VH and VD: New bands in the red region. *Presented by Thomas Varberg.*

**Poster Board #837:** Predicting the properties of early actinide fluorides from advanced electronic structure methods. *Presented by Jackson Maxwell.*

**Poster Board #841:** Computational prediction of pKa and redox potentials for actinides in aqueous media. *Presented by Felipe Dutra.*

**Poster Board #845:** Modelling extraterrestrial photopigments via density-functional theory: Importance and challenges. *Presented by Dorothea Illner.*

**Poster Board #849:** Understanding electron transport in metalloproteins. *Presented by Jitong Ren.*

**Poster Board #830:** Molecular dynamics investigation of deep eutectic solvent structure and properties based on hydrogen bond acceptor variation. *Presented by Jenna Lane.*

**Poster Board #834:** Investigating physical properties of disaccharide-based deep eutectic solvents. *Presented by Jenna Lipani.*

**Poster Board #840:** Reaction pathways for the formation of magnesium oxides from water and metal hydrides. *Presented by Kailey Bell.*

**Poster Board #844:** DNA-Gemini surfactant interactions: Sequence and environmental effects. *Presented by Derek Aguilar.*

**Poster Board #846:** Performance of a hybrid explicitly correlated coupled cluster method for the use in anharmonic vibrationla frequency computations. *Presented by Alexandria Watrous.*

**Poster Board #850:** Sequestration of brilliant green from aqueous solution using composites of reduced graphene oxide with chitosan and chitosan beads. *Presented by Olayinka Oluwasina.*

**Poster Board #929:** Structure-function relationships of conjugated compounds investigated with classical and entangled light for application in quantum sensing. *Presented by Sara Jovanovski.*

**Poster Board #933:** Hydrolysis reaction pathways of early actinide oxide nanoclusters. *Presented by Eddy Lontchi.*

**Poster Board #937:** Efficient and stable self-passivation perovskite solar cells prepared in ambient air based on antisolvent free method. *Presented by Qiqi Zhang.*

**Poster Board #941:** Ultrafast vibrational dynamics of derivatized Lehn's catalyst using transmission-mode 2DIR and development of reflective-2DIR for surface-attached samples. *Presented by Rebecca Hopkins.*

**Poster Board #945:** Computational investigations of the water structure at the  $\hat{1}\pm\text{-Al}_2\text{O}_3(0001)$ -water interface. *Presented by Xiaoliu Zhang.*

**Poster Board #949:** Rovibrational quartic force fields of magnesium Tricarbide-multireference character thwarts a full analysis of all isomers. *Presented by Donatus Atsu Agbaglo.*

**Poster Board #949:** Rovibrational quartic force fields of magnesium Tricarbide-multireference character thwarts a full analysis of all isomers. *Presented by Ryan Fortenberry.*

**Poster Board #928:** Unexplored phases in  $\text{HfO}_2$  from first principles. *Presented by Tianhongyi Zhao.*

**Poster Board #932:** Ab initio characterization of thermal and aqueous stability of near-surface nitrogen-vacancy centers in diamond. *Presented by Sirisak Singesen.*

**Poster Board #936:** Rapid exciton diffusion and structural defects in individual PCN-222 microcrystals. *Presented by Sajia Afrin.*

**Poster Board #938:** Electronic structure of the 3d metal series of mono acetylide cations. *Presented by Nathan Deyonker.*

**Poster Board #942:** Condensed phase dynamics of atmospherically relevant molecules at the air-water interface of organic aerosols. *Presented by Lily Guidry.*

**Poster Board #948:** Vibronic spectroscopy of cyclopentenone isomers in their lowest triplet excited states. *Presented by Alexander Narkiewicz-Jodko.*

**Poster Board #948:** Vibronic spectroscopy of cyclopentenone isomers in their lowest triplet excited states. *Presented by Jenna Trzebiatowski.*

**Poster Board #950:** Ambient STM visualization of self-assembled Cyclopentadienylmolybdenum(ii) tricarbonyl dimers. *Presented by Yen-Chen Chen.*

**Poster Board #1027:** Possible molecular origins of the unidentified infrared emission features in planetary nebulae. *Presented by Thomas Toolis.*

**Poster Board #1031:** Computationally exploring the photochemistry of model brown carbon chromophores. *Presented by Hayden Harkins.*

**Poster Board #1035:** Doping of organic and nanocrystalline semiconductors brings about increased conductivity and quantum yield respectively; also the synthesis of 1D silver Phenyltelluroate allotropes. *Presented by Timothy Atallah.*

**Poster Board #1039:** Molecularly imprinting benzylfentanyl for the detection of fentanyl. *Presented by Geornipha Milbin.*



**Poster Board #1043:** Effect of relative humidity on desorption rates of air contaminants from a model polyester surface. *Presented by Annabel Edwards.*

**Poster Board #1047:** Nuclear-electronic orbital method with kinetic energy constraints. *Presented by Eno Paenurk.*

**Poster Board #1028:** Cocrystallization of long-chain n-alkyl bromide with lipid-like ionic liquids: A case of serendipity. *Presented by Muhammadiqboli Musozoda.*

**Poster Board #1032:** Clock microscopy: Embedding additional information in optical images of single nanoparticles. *Presented by Zachary O'Dell.*

**Poster Board #1034:** Structural and energetic properties of Pd nanoclusters. *Presented by Shane Autry.*

**Poster Board #1038:** Exploring molecular polaritons in the gas phase. *Presented by Jane Nelson.*

**Poster Board #1042:** Potential role of neuronal calcium sensor-1 and DREAM in methyl viologen induced neurotoxicity. *Presented by Michael Reyes.*

**Poster Board #1048:** Three colors, three compounds with different forms of TCNQF4 from a simple chemical system. *Presented by Milagros Tomas.*

**Poster Board #1129:** Systematic investigation of group 13 hydrides: Dramatic changes from boron to thallium. *Presented by Anton Pozdeev.*

**Poster Board #1133:** Exploration into the possible mechanisms that describe dual fluorescence. *Presented by Nicolas Lutfi.*

**Poster Board #1135:** Influence of electronic coupling in the proton-coupled electron transfer of Phenylenediamines. *Presented by Giovanni Parada.*

**Poster Board #1139:** Investigating the effect of water on the mechanical properties of cellulose from multiscale molecular dynamics simulations. *Presented by Meagan Crowley.*

**Poster Board #1143:** Photostability and excited-state features of the natural UV-screening compound vulpinic acid. *Presented by Derek Moore.*

**Poster Board #1147:** Increased triplet separation and transfer rates following singlet fission in perovskite-templated tips-pentacene films. *Presented by Arthur Bragg.*

**Poster Board #1114:** Simulation of polariton dynamics in the Fenna-Matthews-Olson complex. *Presented by Luis Herrera Rodriguez.*

**Poster Board #1116:** Ex-situ synthesis and characterization of PEDOT: PSS-Au NP composite thermoelectrics. *Presented by Won Sung Kim.*

**Poster Board #1120:** Ionic liquids for aqueous stabilization of near infrared dye material. *Presented by Abigail Townsend-Hartline.*

**Poster Board #1124:** Computational characterization of aluminum nitride clusters for interstellar chemistry. *Presented by Jonathan Dotson.*

**Poster Board #1128:** Characterization and enhancement of the photoluminescence of near-IR emitting Cd3P2 quantum dots. *Presented by Logan Smith.*

**Poster Board #1215:** Wacker-type oxidation of diverse aryl-substituted alkenes over Pd(II) organometallic SBA-15 catalyst under microwave. *Presented by Hong Yin.*

**Poster Board #1217:** Fluorinated and chlorinated aluminium and boron molecular rovibrational spectra. *Presented by Irene Bishop.*

**Poster Board #1221:** Conformational studies of perfluorooctanoic acid (PFOA) in the presence of its helicity. *Presented by Ailinh Tran.*

**Poster Board #1225:** Development of ab initio-derived force fields for accurate modeling of silica-CO<sub>2</sub> interactions. *Presented by Sahan Godahewa.*

**Poster Board #1214:** Optimized force field for silica-water interfaces. *Presented by Thanuja Jayawardena.*

**Poster Board #1218:** Exploring the impact of vibrational strong coupling strength on elementary reaction dynamics via ultrafast spectroscopy. *Presented by Liying Chen.*

**Poster Board #1222:** Spatially resolved photothermal infrared spectroscopy of amyloid aggregates in cerebral amyloid angiopathy. *Presented by Ana Gabriela Pacheco de Oliveira.*

**Poster Board #1226:** Evolution of amyloid structure across Alzheimer's disease stages using infrared microscopy. *Presented by Brooke Holcombe.*

**Poster Board #1313:** Prediction of key products in  $\beta$ -pinene ozonolysis. *Presented by Jeff Wang.*

**Poster Board #1317:** Stability of two-dimensional MoS<sub>x</sub>(x=2-3) through structural optimization. *Presented by Abu Asaduzzaman.*

**Poster Board #1319:** Nanoscale infrared spectroscopy reveals the morphology and structure of individual co-aggregates of amyloid beta and Amylin. *Presented by Siddhartha Banerjee.*

**Poster Board #1321:** Photothermal infrared microscopy of amyloid aggregates in Alzheimer's disease. *Presented by Will Chase.*

**Poster Board #1325:** Developing structure-function relationships for the design of optoacoustic imaging probes. *Presented by Carly Wickizer.*

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