

FALL 2026 ACS MEETING

Division of Physical Chemistry POSTER SESSION

Prof. Bern Kohler, *Organizer*

Tuesday, August 25 | 6:00pm – 8:00pm

McCormick Place Convention Center

Hall F2 - POSTERS

Poster 1595. Potential path for the formation of PAHs in deep interstellar space: Exploration of the indenyl and benzyl radical reaction. **S. Arias**, A.M. Mebel

Poster 1596. Ultrafast thermal spectroscopy of interfacial energy transfer. **S. Zare**, J. Maria, J.D. Caldwell, P. Hopkins

Poster 1597. Spectroscopic signatures and nonradiative decay in excited states of caffeine and theophylline. **V.B. Singh**

Poster 1598. Electron bridges for balancing the activity–stability trade-off in electrocatalysis. **X. Han**

Poster 1599. Role of electrolyte entropy in the slow dielectric dynamics at charged electrode interfaces. **H. Fang**, Z. Fakhraai

Poster 1600. For molecular polaritons, disorder and phonon timescales control the activation of dark states in the thermodynamic limit. **T. Li**, A. Montoya Castillo

Poster 1601. Temperature dependent spin relaxation dynamics in achiral and chiral perovskite quantum dots. **M. Khvichia**, D. Zeitz, C. Todd, Y. Ping, J.Z. Zhang

Poster 1602. Rare-Earth-modified luminescent two-dimensional nanosheets derived from oxidized Mo_2CT_x MXene. **S.K. Kurumbara Arachchige**, C. Chen, A. Dutta, A. Kuzmin, F. Yao, P.N. Prasad

Poster 1603. Local electrostatic potentials enable accurate and efficient prediction of water dissociation constant and reduction potential of water in aqueous electrolytes. **A. OZKANLAR**, A.E. Clark

Poster 1604. Strong field ionization and dissociation dynamics of vinyl bromide ($\text{C}_2\text{H}_3\text{Br}$) initiated by few-cycle pulses. **T. Olowolafe**, G. Adusei, D. Mukherjee, A. Durden, S. Abubakar, B. Oguh, A. Udoikono, S. Lee, H.B. Schlegel, W. Li

Poster 1605. Room temperature size tuning of quantum dots for photocatalysis. **M. Mukherjee**, P.V. Kamat

Poster 1606. Unraveling the key determinant underlying the critical phosphate release step of an ATPase. **K. Herman**, S. Sridharan Iyer, Y. Wang, T. Pollard, G.A. Voth

Poster 1607. Ultrafast relaxation pathways in N,N'-dimethyl indigo probed by femtosecond absorption spectroscopy. **N.S. Muir**, A.B. Pun, H. Yong

Poster 1608. Synergistic excitonic and plexcitonic processes in Organic-Quantum Dot and Plasmonic hybrids: Novel nanomaterials for rethinking triplet photophysics. **S. Rawool**, A.J. Ayitou

Poster 1609. Multidimensional attosecond spectroscopy reveals spin-vibronic couplings and many-body correlations in charge transfer materials. **J. Higgins**, J.D. Gaynor

Poster 1610. Nitroxide-doped anionic micelles as model systems for quantum sensing. **A. Laaj**, C.A. Totoiu, P.H. Oyala, D.A. Dresios, R. Hadt

Poster 1611. Controlling biexciton transport in molecular aggregates influenced by exciton–exciton annihilation. **R. Dutta**, C. Chuang

Poster 1612. Concentration-dependent ion mobility in aqueous LiCl: New insights into hopping vs. vehicular transport. **S. Paul**, A.E. Clark

Poster 1613. Coherent vibrational dynamics near conical intersections for light harvesting. **C. Leslie**, W.F. Beck

Poster 1614. Ultrafast electron relaxation dynamics in plasmonic nanostructures. **Y. Wu**, G.C. Schatz

Poster 1615. High-pressure induced activation of AsLOV2 stabilizes triplet spin state. **R. Han**, S. Maity, L.L. Gardner, S.D. Jacobsen, S. Han

Poster 1616. Dynamics of surface-tethered DNA across materials, coatings, applied voltage, and ion concentration: A comprehensive all-atom molecular dynamics study. **Y. Noh**, H. Chang, K. Fu

Poster 1617. Water-network disorder determines the vitrification concentration in cryopreservation solutions: A mechanistic study. **E. Lee**, N. Gaby-Biegel, R. Sandlin, C. Baiz

Poster 1618. Controlling excited state intersystem crossing in pyrazolate-bridged Pt(II) dimers by excitation photon energies. **W. Chen**, M. Taub, S. Kromer, X. Li, F.N. Castellano, L.X. Chen

Poster 1619. Predictive model for transition metal oxide photocatalyst lifetimes derived from experimentally measured polaron parameters. **Y. Cao**

Poster 1620. Multiscale computational modeling of FtsZ protein assembly in bacterial cell division. **Y. Luo**, J. Mannik, Y. Qiu

Poster 1621. Size-dependent effects of a hydrophobic solute on water structure and dynamics. **N. Uzoukwu**, W.H. Thompson

Poster 1637. Breaking the mobility–reliability trade-off in IGZO transistors via interfacial Ga₂O₃ engineering toward next-generation DRAM cell transistors. **T. LEE**, H. Jang

Poster 1638. Dynamics and spectroscopy of excess electrons in binary ionic liquid mixtures. **D. Das**, k. Huber, M. Knudtson, D.A. Blank, J.F. Wishart, C. Margulis

Poster 1639. Mid-IR asynchronous and interferometric nonlinear spectroscopy of low-fluence band-edge dynamics in narrow-gap semiconductors. **H. Jang**, G. Han, M. Cho

Poster 1640. High-throughput, rapid, automated optical characterization of perovskite photovoltaics: Stability testing and device insights. E. Schwartz, A. Louks, A. Troupe, B. Motes, Z. Han, A. Palmstrom, Q. Jiang, J. Berry, J. MacKenzie, **M. Hasham**

Poster 1641. Evolution of plasmonic and magnetic properties of F-Cd₂SnO₄ nanocrystals with size. **S.D. Bennett**, G.F. Strouse

Poster 1642. Probing Boltzmann-trapped quintet multiexcitons in singlet-fission materials at high magnetic fields and ultra-low temperatures: Toward the pure polarization limit. **H. Le**, Q. Stern, S. Han, S. Patil

Poster 1643. Spectroscopic investigation of pH-dependent photophysics in amino acid–functionalized meso-modified cyanine dyes. **N. Azizi Khereshki**, M. Henary

Poster 1644. Organic molecular color center qubits as platforms for quantum sensing. **S. Kopp**, Y.R. Poh, J.R. Palmer, K.R. Peinkofer, B.P. Phelan, S. Nakamura, P. Watts, J. Yuen-Zhou, M. Krzyaniak, M.R. Wasielewski

Poster 1645. Variation of surface propensity of halides, alkali ions and ion-pairing from supercooling to above room temperature. **S. Consta**

Poster 1646. Synthesis and photophysical investigation of substituted ruthenium(II) bis(2,6-di(quinolin-8-yl)pyridine) complexes. **A.M. Jamhawi**, J.A. Bella, D.A. Modarelli

Poster 1647. Paramagnetic dopants enable endogenous polarization for pulsed DNP solid-state NMR of inorganic materials. **L. Zhu**, D. Zhang, Y. Quan

Poster 1648. Ultrafast charge, spin, and lattice dynamics and coupling in metal semiconductors. **A. Partin**, H. Gajapathy, S. Biswas, L. Baker

Poster 1649. Solid-state organization and excited-state photophysics of covalently stapled chiral perylene diimide polymers. **J. Maleszka**, I. Tsironi, A. Jones, J. Olivier

Poster 1650. Probing the effects of environment on novel CCC-NHC-Pt(II) pincer complexes. **C. Brower**, N. Kruse, M. Zhang, C.E. Webster, T.K. Hollis, N. Hammer

Poster 1651. Spectroscopic and quantum chemical investigation of molecular clusters involving battery electrolytic co-solvents. **K. Arnett**, N. Hammer

Poster 1652. Triplet exciton dynamics in CdSe quantum dots functionalized with arene carboxylates. **M. Dinesh**, S.A. Shameem, W.F. Beck

Poster 1653. Quantum transport signatures of polaritonic states in molecular cavity QED systems. **J. Klein**, J. Bergfield

Poster 1654. Identifying quantum interference effects from joint conductance-thermopower statistics. **J. Bergfield**

Poster 1655. Stabilizing effect of neighboring disordered RGG domain on the folded state of FUS-RRM. **K. Rahimi**, A. GUPTA, K. Malekzadeh, G. Zerze

Poster 1656. Modeling the photophysics of novel molecular light-to-heat converters. **J.M. Toldo**

Poster 1657. Characterizing the coherence of single perovskite quantum dots. **E. Daggett**, L. Huang, J. Hood

Poster 1658. Infrared nanospectroscopy of dynamic processes in liquids. **A. Danilov**, K. Kaltenecker, F. Weston

Poster 1659. Vibronic coherences in photoinduced charge transfer from CdSe quantum dots to surface-bound acceptors. **S.A. Shameem**, N. Mohan T M, C. Leslie, C.V. Hetherington, B.G. Levine, W.F. Beck

Poster 1660. Disentangling exciton fission, transport, and annihilation dynamics in N,N'-bis(2-phenylethyl)-3,4,9,10-perylenedicarboximide crystals. **T.S. Volek**, S.T. Roberts

Poster 1661. Structural asymmetry and charge segregation drive helical supramolecular assembly in zebrafish germ plasm condensates.

A. Tabares-Brown, D.A. Olaya Muñoz, J.P. Hernandez Ortiz, F.J. Pelegri

Poster 1662. Conferences in color: Visual note taking as a way of capturing oral presentations. **O.H. Wilkins**

Poster 1663. Molecular materials for light-driven charge accumulation. **D. Bain**, J.T. Yarranton, T.N. Haddock, L.X. Chen

Poster 1664. Incoherent mixing background removal in photocurrent-detected two-dimensional electronic spectroscopy. **A.B. Gilbert**, Z.M. Faltz, D. Im, C.J. Blackwell, M.S. Arnold, M.T. Zanni

Poster 1665. Sn_2TiO_4 -based dye sensitized solar cells: TCNQ-oxide systems as a test case. **A.R. Flint**, G.R. Jenness, M.K. Shukla

Poster 1666. Decoupling coherent electron phonon interactions in metal organic chalcogenides. **H. Yang**, W. Shao, Y. Cai, M. Chen, L. Dou, L. Huang

Poster 1667. Oxidized eumelanin model compounds: Ultrafast excited-state dynamics of an indole quinone dimer. **R. Pozza**, W. Bouthillier, A. Manickoth, L. Blancafort, J. Lumb, B. Kohler

Poster 1668. Subspace corrections to quantum ansätze for molecular ground state calculations. **P.F. Kwao**

Poster 1669. Near-unity triplet quantum yield in an organic molecular H-dimer. **M.C. Drummer**, R. Sun, A. Florescu-Ciobotaru, D.G. Nocera

Poster 1670. Insight into the adsorption and inhibition mechanism of pyrazole derivatives as highly efficient inhibitors for carbon steel: A combined electrochemical, surface, and DFT/MD study. **A. BARRAHI**, N. TIMOUDAN, L. CHAHIR, A. Marzaq, r. saddik, S. Tighadouini, F. Benhiba, B. Dikici, A. Zarrouk

Poster 1692. Understanding and perturbing the aggregation behavior of large phosphate clusters. **E. Uyar**, A.E. Clark

Poster 1693. *In situ* observation of stimulus-dependent degradation pathways in metal halide perovskites via light-coupled atmospheric gas-cell TEM. **K. Saidov**, P. Nandi, Z. Cai, M.G. Kanatzidis, V.P. Dravid, D. Swearer

Poster 1694. Multiscale *in silico* modeling of lactate dehydrogenase (LDH) structure and assembly. **K. Alonso**, S. Chatterjee, K. White, J.K. Whitmer

Poster 1695. Solvent dependent dark state pathways in Cyclohexyluracil: Twisted ground state intermediate versus $1n\pi^*$ state. **T. Tonny**, R. Mathew, C. Crespo-Hernández

Poster 1696. Moiré beyond van der Waals: Twist-angle-dependent exciton diffusivity and temperature dependence in twisted MAPbBr₃. **S. Chen**, J. Li, L. Huang, L. Dou

Poster 1697. Plasmon-enhanced exciton transport in complex nanophotonic environments: Insights from quantum dynamics simulations. **G. Liu**, H. Chen

Poster 1698. Developing magnetic circularly polarized luminescence (MCPL) spectroscopy to elucidate excited-state electronic structure. **N. Kazmierczak**

Poster 1699. Optical control of spin dynamics in a single pentaazaphenylene molecule with singlet-triplet inversion. **Y. Shang**, A. Fairhall, K. Wilson, R. Young, A. Nguyen, P. Maurer, M.R. Wasielewski, E. Garand, R.H. Goldsmith

Poster 1700. Bath-driven formation and control of decoherence-protected excitonic subspaces in perovskite quantum materials. **P. Kambhampati**

Poster 1701. New water oxidation mechanism in Photosystem II resolves major experimental controversies. **Y. Pushkar**

Poster 1702. ZnO quantum dot–molecule conjugates: Chemical interactions, charge dynamics, and spin polarization. **J.H. Olshansky**

Poster 1704. Role of Li⁺ ions in polyzwitterionic ionogels: Gelator or Mobile charge carrier?. **S. Arwish**, M. K. Alsaedi, R. P.O Hara, A. Asatekin, M. Panzer, M. Schonhoff

Poster 1705. Four-component multireference perturbation theory within the small tensor product distributed active space (STP-DAS) framework. **R.S. Majumder**, S. Upadhyay, M. Oele, X. Li

Poster 1706. Real-time visualization of molecular diffusion and dynamics during the ripening of ATP condensates. **F. Chen**, A. Moussavi, C. Rademacher, S. Keten, D. Ercek, M. Wang

Poster 1707. Low temperature molecular spin decoherence dynamics using Lindblad master equation method. **K.E. Coffin**, T. Krogmeier, K. Head-Marsden, A.W. Schlimgen

Poster 1708. Magneto-optical enhancement in hybrid nanostructures: Interplay of plasmonic, chiral, and doped semiconductor systems. **A. Dutta**

Poster 1709. Strong non-radiative recombination driven by hybrid halogen plane interstitials in α -CsPbI₂Br perovskites. **X. Li**

Poster 1710. 2D electronic-vibrational spectroelectrochemistry: Vibronic coupling in organic mixed conductors. **G. Christenson**, J.D. Gaynor

Poster 1711. Restoring ferroelectricity in Ba-Doped BiFeO₃ *via* topochemical fluorination: A route to switchable *P4mm* multiferroics. **A. Kamigaito**, K. Shigematsu, M. Kobayashi, K. Amemiya, H. Kumigashira, T. Katayama, A. Chikamatsu

Poster 1712. Corrosion inhibition performance of benzimidazole derivatives for protection of carbon steel in hydrochloric acid solution. **N. TIMOUDAN**, A. BARRAHI, L. CHAHIR, L. El Foujji, B. Dikici, F. Benhiba, R. Bouhfid, F. Bentiss, A. Zarrouk

Poster 1713. Impact of structural variations on electronic structure, charge transport, and dielectric properties of porphyrin-based COFs. **A. Maghfori**, Y. Wang, B. Neupane

Poster 1714. Thermodynamically consistent modeling of decoherence in molecular-scale transport. **E. Erdogan**, J. Bergfield

Poster 1715. Band hybridization effects on hot-carrier dynamics in ternary alloys. **L. Rojas**, K.M. McPeak

Poster 1716. Monolayer films of cobalt–aluminum oxide nanoparticles for carbon nanotube synthesis. **B. Regmi**, I. Wickramasuriya, B.S. Guiton, N.T. Alvarez

Poster 1717. Chirality-dependent rare earth ion transport and separations in carbon nanotube porins. **J. Abdullah**

Poster 1718. Spin-labeled nanodiamond as a biocompatible polarization agent to external analytes. **Z. Gao**, J. Straub, S. Han

Poster 1719. Contact-accessible silver nanoparticle-decorated electrospun carbon fibers for microplastics detection by SERS. **F. Joshua**, Y.Y. Li Sip, A. Biswas, V. Gray, D. Chanda, L. Zhai

Poster 1720. Computational Investigation of Radical-Driven Cyclization of Acrylonitrile on Titan and in Astrochemical Environments. **A. Hartwig**, A.M. Mebel

Poster 1721. Antioxidant activity of synthetic eumelanin exposed to UVA radiation. **R.H. Mitchell**, B. Fornaciari, B. Kohler

Poster 1722. Sticking probabilities of structural isomers of butene under non-equilibrium gas-surface collision conditions. **F. Lizano**, E.A. Jamka, S.J. Sibener

Poster 1723. Quinone contributions to optical properties of natural organic matter and DOPA melanin revealed by electrochemical and chemical reduction. **A. Beyhaqi**, B. Poulin, B. Kohler, G. McKay

Poster 1724. CO and N₂ produced from cometary ice analogs. **A. McKinnon**, A. Simon, M. Brann, E.L. Piacentino, K. Oberg, M. Rajappan

Poster 1725. Electron-Stimulated Desorption of the trihydrogen cation: "The molecule that made the universe". **S. Swaminathan**, C.R. Arumainayagam

Poster 1726. Subspace Field Theory 1: Derivation of Planck's Constant. **B.C. Dian**

Poster 1727. Automated refinement of atmospheric chemical reaction models using *ab initio* quantum chemistry. **C. Liao**, M. Reiher

Poster 1728. Accurate quantum chemical exploration of diffusion of radicals on astrochemical grains. **M. Upadhyay**, P. Bera

Poster 1729. Iron-doped CsPbBr₃ nanocrystals for magneto-optical applications. **C. Valdes**, Z. VanOrman

Poster 1730. Probing molecular interactions at liquid-liquid phase boundaries via Raman spectroscopy. **A. Berke**, C. Klurfeld, L. Mintz, Y. Ma

Poster 1731. Characterizing celecoxib crystalline polymorphs with terahertz spectroscopy. **T.F. Akinode**, T.M. Korter

Poster 1732. Spectroscopic insights into second coordination sphere waters in Gadolinium contrast agents: implications for relaxivity and dynamic nuclear polarization. **M. Judd**, P.E. Doan, B.M. Hoffman, S. Han

Poster 1733. Coupled multi-proton dynamics near a lipid membrane. **H. Zhang**, G.A. Voth

Poster 1760. Enhanced Nonlinear Optical and Time-Resolved Properties of Noble Metal Nanoclusters. **H. Geiss**

Poster 1761. Probing the optical properties of polymeric carbon dots: A TD-DFT study of candidate molecular fluorophores. **J. Duchimaza Heredia**

Poster 1762. Overcoming membrane fouling in water purification: A comprehensive approach. **Y. Ezaier**, A. HADER

Poster 1763. Investigating the quantum optical properties of conjugated dye molecules for medical imaging. **R.A. Schmidt**, T.G. Goodson

Poster 1764. Electrochemical growth of water tolerant Zn based MOF coatings for structured CO₂ capture sorbents. **A. Martinez**

Poster 1765. Imaging quantum interference in molecular junctions with spatially resolved thermopower. **H. Jilek**, J. Bergfield

Poster 1766. High sp³ defect density induces axial quantum confinement in single-walled carbon nanotubes. **Z. Zhulficar**, J. Fortner, E. Afriyie, Y. Wang

Poster 1767. Study of NH + NO₂ under conditions representative of hot exoplanet atmospheres. **Z. Auvil**

Poster 1768. Molecular spectroscopy for space and planetary science. **A. Mattioda**, K.M. Yocum, A. Vats, G. Schlick, C. Dang, E. Quigley, M. Jordan

Poster 1769. Nanodiamond-based multidimensional sensing technique for metabolite identification. **E. Brown**, G. Geng, A. Ajoy

Poster 1770. Vibrational signatures of hypervalent iodine macrocycle: Exploring coupling and electronic effects using FTIR and 2D IR spectroscopy. **R. Krishnan**, S. Arafin, T. Awais, M. Kersten, K.E. Helme, K.N. Plunkett, S.D. Moran

Poster 1771. Quantum cavity control of electron transfer: non-monotonic collective effects and cavity-modified light-matter interactions. **S. Sharma**

Poster 1772. Highly multiplexed and fast single molecule localization microscopy. **B. Dong**

Poster 1773. Photophysical properties of tunable DOX-IR820 chemo-PTT combination nanomedicine. **E. Nadeem**, F. Abbas, N. Siraj

Poster 1774. Spin-correlated radical pairs as potential precursors of TADF: Probing spin dynamics and magnetic field effects. **K. Bortey**, R.J. Vazquez

Poster 1775. Electrochemical kinetics and mechanistic analysis of a thiol-functionalized cobalt porphyrin in aqueous media. **G. Seiden**, U. Udeochu

Poster 1776. In-liquid infrared near-field nano-spectroscopy modeled using a near-field to far-field transformation. **I. Kats-Rodgers**, E.A. Muller

Poster 1777. Phase-resolved near-field infrared microscopy approaching the shot-noise limit. **P. Rizzo**, E.A. Muller

Poster 1778. Investigating thermodynamic origins of the change of specific heat capacity in polymer–lanthanide chelation. **C.C. Armstrong**, J. Mase, M.D. Schulz

Poster 1779. Effective surface passivation of CsPbBr₃ quantum dots via post-synthetic treatment with zwitterionic and quaternary ammonium salt ligands. **J. JO**, J. Yang

Poster 1780. Computational investigation of thermodynamic stability in novel high entropy MAB phases based on the Cr₄AlB₄ structure. **U.A. Adhikarige**, D. Cakir

Poster 1781. Electron–phonon coupling governing spin and hot carrier dynamics in 2D perovskites. **Y. Huang**

Poster 1783. Improved method to determine the THz refractive index of materials. **W. Hom**, J.A. Johnson, M. Lutz, G. Phillips

Poster 1784. Plasmonic nanogap enhanced 2H to 1T' phase transition in MoTe₂. **B.S. Siriwardana**, O. Shaibu, O. Savkina, B.M. Rajapakse, J. Bird, P.N. Prasad, L.A. Velarde

Poster 1785. Anisotropic ferroelectric switching and grain boundary effects in BaTiO₃: an atomistic study. **S.T. Folarin**, S. Manna, S. Subramanian

Poster 1786. Computational studies of membrane structure and pPermeability by PIP₂, cholesterol, and ceramide 18 in a heterogeneous neuronal lipid bilayer. **R. Versace**, **A. Urbina Morales**

Poster 1787. Characterizing the anharmonic coupling of the OH stretching mode in 10-Hydroxybenzo[h]quinoline using constrained nuclear-electronic orbital theory. **H. Newton**, Y. Wang, Y. Yang

Poster 1788. Ultrafast vibronic dynamics and charge-carrier localization in bismuth halide perovskites. **P.N. Carlson**, P. Kodimana Ramakrishnan, J.D. Gaynor

Poster 1789. Native and apo- α -Lactalbumin binds to anionic mixed liposomes showing differential insertion depths. **A. Sayeed**

Poster 1790. Temperature effects on green-synthesized iron oxide nanostructures. **A. Hancock**, D. Torres

Poster 1792. Comparison of linear and branched Poly (ethylene glycol) in preventing Nonspecific binding of DNA on glass substrate. **U. Umaru**, J. Chen

Poster 1793. Investigating chiral contributions to electronic-vibrational interactions with multidimensional spectroscopy. **A. Seys**, B. Hou, M.K. Shehab, O. Farha, J.D. Gaynor

Poster 1794. Unified quantum-dynamic framework for predicting circularly polarized emission in chiral π -conjugated polymers. **K. KEYA**, D. Kilin

Poster 1795. Ultrafast structure-dynamics relationship of Pt(IV) based near-IR triggered bioactive molecules. **M. Pandey**, M. Kshetri, Y. Zheng, A. Konar

Poster 1796. Exploring iron bearing Martian minerals using terahertz spectroscopy and density functional theory. **A. Cary**, T.M. Korter

Poster 1797. Anthraquinone-based multifunctional additive for efficient defect passivation and enhanced electronic coupling in high-performance perovskite solar cells. **G. Yoon**, J. Jung

Poster 1798. Conformation-dependent electronic properties of aromatic amides. **Y. Kidokoro**, R. Samajda, X. Liu, K. Kuyama, F. Takeda, I. Okamoto, M. Kawahata, K. Katagiri, J.S. Moore, C. SCHROEDER, A. Tanatani

Poster 1799. Mitigating surface defects and interfacial trap states at nickel oxide hole-injection layers via self-assembled monolayers for efficient blue perovskite light-emitting diodes. **J. Song**, J. Jung

Poster 1800. Strong interfacial coupling of a self-assembled monolayer enables stable and efficient lead-free near-infrared perovskite light-emitting diodes. **J. Yi**, J. Jung

Poster 1801. Coumarin: A multifunctional organic dye for stabilizing grain boundaries and defects in perovskite films for high-performance solar cells. **G. Ku**, J. Jung

Poster 1802. Influence of zero-point sampling on attosecond transient absorption spectra. **S.H. Dinshaw**, L. Kurkowski, K. Lopata

- Poster 1803.** Mn-doped ZnO quantum dots conjugated with organic dyes as hosts for spin-correlated radical pairs. **R. Lin, S. Cho,** A. Jain, J.H. Olshansky
- Poster 1804.** Mapping correlated electron dynamics in iron oxide. **S. Mersch,** J. Higgins, G. Christenson, P. Seliya, J.D. Gaynor
- Poster 1805.** Thermodynamic kinetics of gold ion retrieval by Cross-linked Polyethyleneimine Networks. **M. Sah,** Z. Peng, P. Tao, X. Chen
- Poster 1806.** Deep-energy-level anthraquinone monolayers: Tailoring the interface for efficient deep-blue perovskite electroluminescence. **C. LEE,** J. Jung
- Poster 1807.** New measurements of the product state distributions from Huggins band photochemistry. **M.E. Fast,** D. Lu, H. Guo, S.W. North
- Poster 1808.** Overcoming fluorescence in time-resolved sum frequency generation spectroscopy of organic pollutants using a spatial filter. **E.L. Foss,** B.M. Luther, J.D. Cyran
- Poster 1809.** Two-photon polarization ratio explains unusual shape of the two-photon absorption spectra of fluorescent dyes and detects weak excitonic coupling in fluorescent protein dimers. **M. Drobizhev,** A. Cusick, A. Thuen, S. Schultz, H. Puhl, K. Hines, Y. Kim, S.S. Vogel
- Poster 1810.** Investigating molecular orientation and interfacial chemistry of polymer-coated perovskite single crystals via sum-frequency generation spectroscopy. **P. Ariyaratne,** D.C. Garza, M.E. Kordesch, K.A. Cimat, J. Chen
- Poster 1811.** Implementing finite-element electrochemical simulations in the undergraduate chemistry curriculum. **S. Stenberg,** P. Kumar, R. Resheske, A. Farsi, W. Gao, F. Brushett, S. Sen
- Poster 1812.** neMD/MC Constant-pH simulations reveal state-dependent protonation profiles in channelrhodopsin Chrimson. **S. Moe**
- Poster 1813.** Insights on correlated electron density with topological data analysis. **B. Rakshit,** P.M. Zimmerman
- Poster 1814.** Molecular dynamics of zipper-type imidazolium-bis(trifluoromethanesulfonyl)imide Ionic Liquids at Ag(001) electrodes. **K. Wang,** C. Margulis, S.K. Shaw
- Poster 1815.** Effect of unsaturations in the permeability of ceramide skin lipids. **R. Versace,** D. Gorcowski

Poster 1816. Magnetic Exchange and spin delocalization in acene bridged Blatter radical dyads: A computational study. **D.B. Lawson**

Poster 1817. Enhancing magnetic light-matter interactions in molecular systems. **J. Rios-Narciso**, A.E. Khan, M. Biswas, U. Manna

Poster 1818. Temperature-dependent hydration layer dynamics of distinct conformations in antifreeze glycoprotein-8. **R. Centeno**, K.V. Krishnan

Poster 1819. Real-time observation of polaron formation and its role in cooperative quantum response in perovskite quantum dots. **F. Priya**

Poster 1820. Distinct tubulin C-terminal tails control the efficiency of a microtubule severing machine. **M. Ranpati Dewage**, S. Kahawatte, R.I. Dima

Poster 1821. Ultrafast excited state dynamics of donor acceptor thermally activated delayed fluorescence systems. **J.A. Jerome**, B. Pokhrel, S.R. Rather

Poster 1822. First results of H₂O densities of H₂O ices at 10 – 150 K using microbalance – with refractive indices and Infrared band strengths. **Y. Yarnall**, R.L. Hudson

Poster 1823. Synthesis and photoluminescence quenching kinetics of CsPbBr₃ perovskite nanocrystal-reduced graphene oxide heterostructures. **F. Khan**, T. Khan, N. Arif

Poster 1824. Expanding ultra-coarse-graining to multi-species systems: A systematic bottom-up framework for binary mixtures with state-dependent interactions. **T.S. Qu**, P.G. Sahrman, M. Gerry, G.A. Voth

Poster 1825. Linearized pair-density functional theory for excited-state photocatalytic dynamics. **H.S. Clifford**, A. Seal, A. Cusumano, L. Gagliardi

Poster 1826. Effect of electric fields on dissociation of acidic molecules. **M. Grace**, A. Datar

Poster 1827. Infrared signatures of electric fields and protons in CO–H₂O Complexes. **L. Hatton**, A. Datar

Poster 1828. Proton structure and transport in ionic liquid–water mixtures with varying anion hydrophilicity. **J. Choi**, G.A. Voth

Poster 1829. Photophysical characterization of bismuth–nickel complexes for photocatalytic CO₂ reduction. **C. Liu**, O. Pearre, G. Hu, S.E. Sanders

Poster 1830. Surface enrichment of components in amorphous solids and the effect of acoustic vibrations. **E. Jackson**, B. Upson, M.D. Ediger, L. Yu

Poster 1831. Charge trapping in metal oxides: Insights from transient absorption spectroscopy. **I. Vargas-Hurlston**, C. Johnston, E.P. Craddock, R. Speelman, C. Bridgewater, N.G. Puskar, A. Arcidiacono, S. King

Poster 1832. Electric field modulation of catalysis in liver alcohol dehydrogenase. **J.C. Eze**, J. Gascon

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