# SoCal TheoChem 9

THEORETICAL CHEMISTRY SYMPOSIUM

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| CSU The California State University CSUBIOTECH | QCHEM Fast, Accurate, Robust Molecular Modeling | SDSU College of Sciences Department of Chemistry & Biochemistry |
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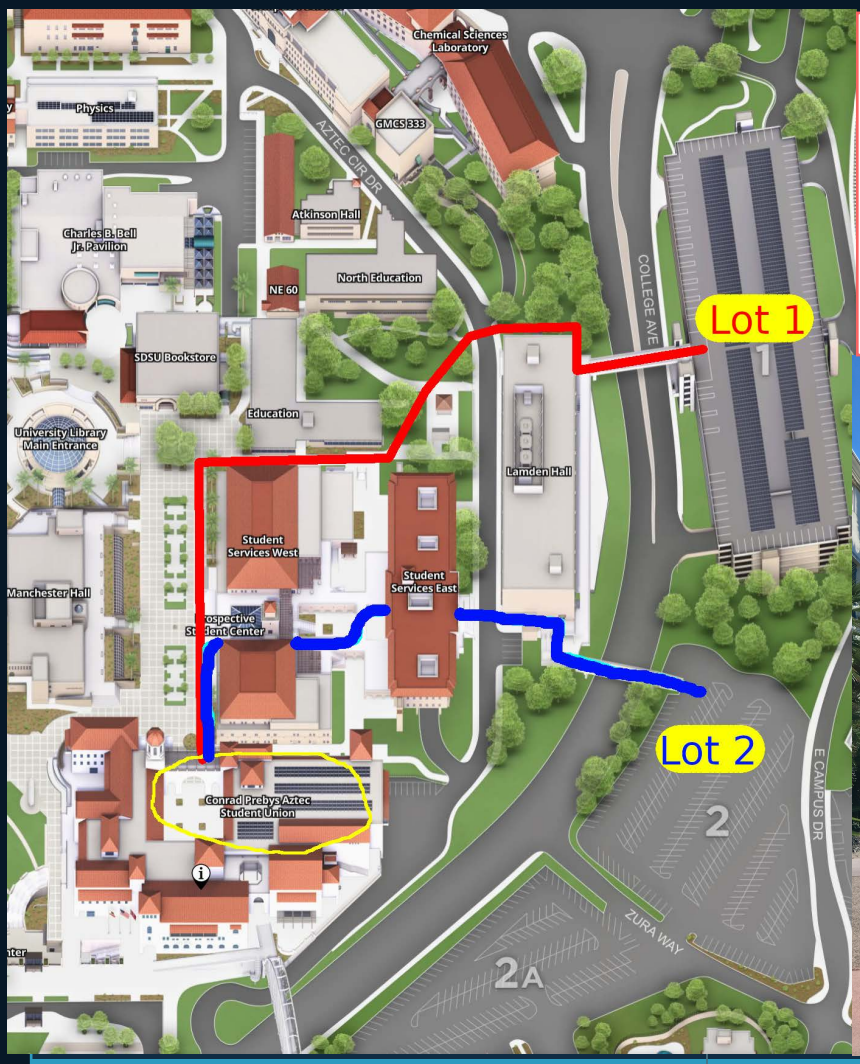
# Campus Map & Parking

The symposium is hosted at the Conrad Prebys Aztec Student Union. Lots 1 and 2 are highlighted below.
For those arriving by trolley, the Student Union is adjacent to the SDSU transit center and trolley station.




- After parking in Lots 1 or 2, cross the bridge over College Ave.
- Go up the stairs at the end of the bridge and cross Aztec Circle Drive.
- Walk west towards the center of campus.
- When you reach the broad walkway, turn left and walk up to the Aztec Student Union.
- Registration, poster session, and talks are on the second floor.



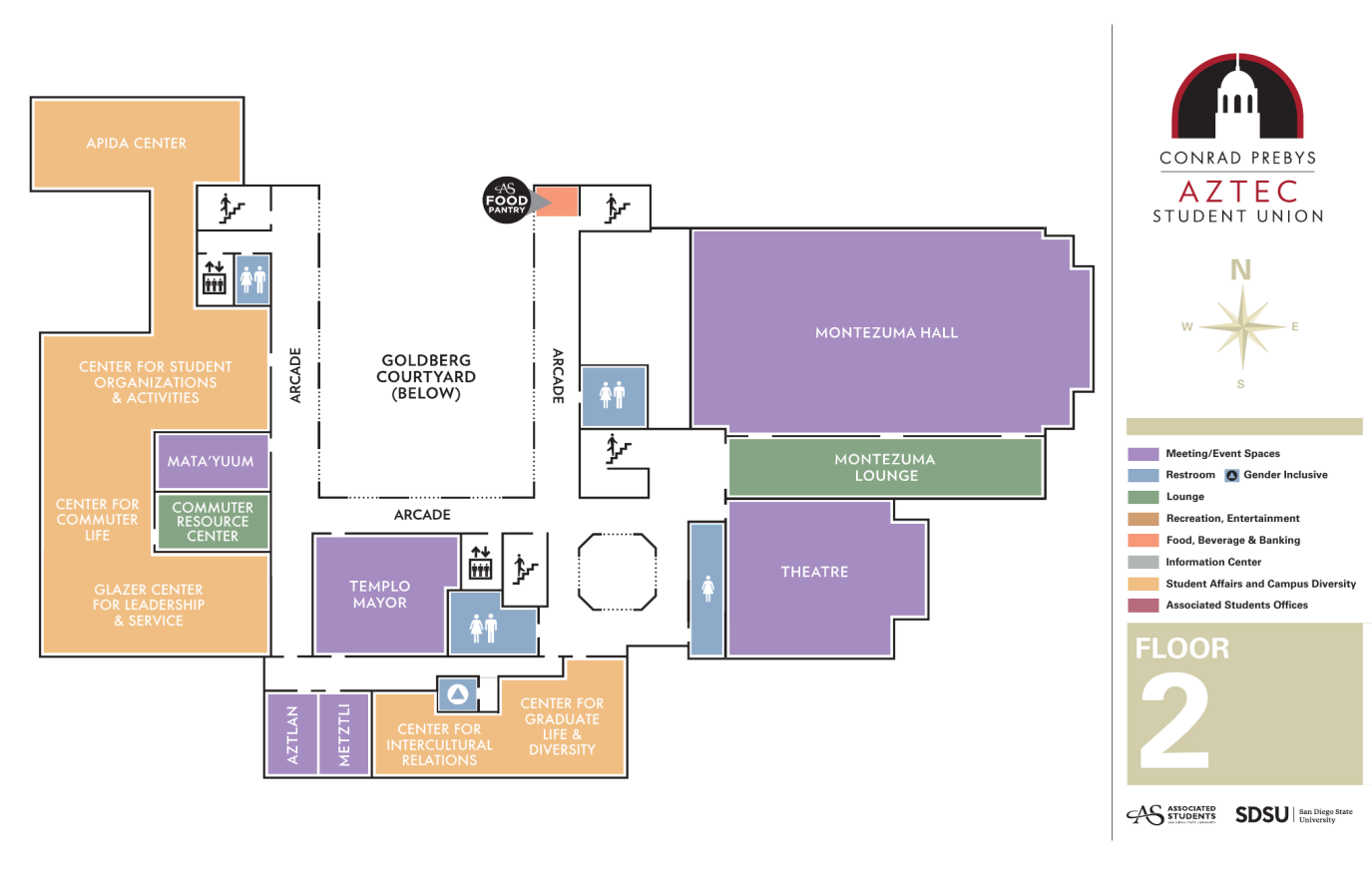
**Attendees who received a parking pass by email and registered their vehicle do not need to pay for parking. All others must pay for parking.**

Parking Information for the Student Union

- Closest Structures: Parking Structure 1 (P1) and Parking Lot 2 (P2). You can park on multiple levels of P1. Park near the top to be close to the bridge over College Ave, or take the elevator to the top floor.
- If you must pay for parking (you do not have a permit): Daily Choice Rate: $4.25 per day (including fees).
- Payment Methods: Permits must be purchased digitally through the Aztec Parking Portal, the PayByPhone mobile app, or on-site pay stations.
- Enforcement: Parking is enforced 24 hours a day, 7 days a week across all campus lots and structures.

# Student Union Floorplan

Use the second-floor plan to move between Union Theater, Templo Mayor, and Mata'yuum.




| UNION THEATER | TEMPLO MAYOR | MATA'YUUM |
|---|---|---|
| Speaker sessions | Poster set-up and poster session | Registration and poster session |

Breakfast, break refreshments, and lunch will be served on the 3rd floor terrace.
Seating is available throughout the Union, including a dining common at the southwest corner of the first floor.

# Program | Morning Sessions

Saturday, November 7, 2026 | San Diego State University Student Union

| TIME | PROGRAM | LOCATION |
|---|---|---|
| 8:00-8:55 am | Registration | Mata'yuum |
| 8:00-8:55 am | Breakfast pastries and drinks | Union 3rd Floor |
| 8:00-8:55 am | Poster set-up | Templo Mayor / Mata'yuum |
| 8:55-9:00 am | Welcome | Union Theater |
| 9:00-9:30 am | **Zhenglu Li, USC**: Correlated excitations across space and time: Electron-phonon interactions, Wigner crystalline excitons, and ultrafast nonequilibrium dynamics | Union Theater |
| 9:30-10:00 am | **Kieron Burke, UC Irvine:** Density Functional Theory: From the mundane to the outer limits | Union Theater |
| 10:00-10:20 am | Coffee break | Union 3rd Floor |
| 10:00-10:20 am | Poster set-up | Templo Mayor / Mata'yuum |
| 10:20-10:50 am | **Wanlu Li, UC San Diego:** Short-Range Order as a Design Variable for Complex Multielement Electrocatalysts | Union Theater |
| 10:50-11:20 am | **Vincent Esposito, Chapman University:** Computational astrochemistry - from the spectroscopy and formation of PAHs to interstellar photochemistry | Union Theater |
| 11:20-11:40 am | **Kimberly Daas, UC Irvine:** Ensemble Time Dependent Density Functional Theory | Union Theater |
| 11:40 am-12:00 pm | **Arnab Chakraborty, USC:** Tracking the Evolution of Electronic Character of Ground and Excited States with Mixed-Reference Spin-Flip TDDFT | Union Theater |

# Program | Afternoon Sessions

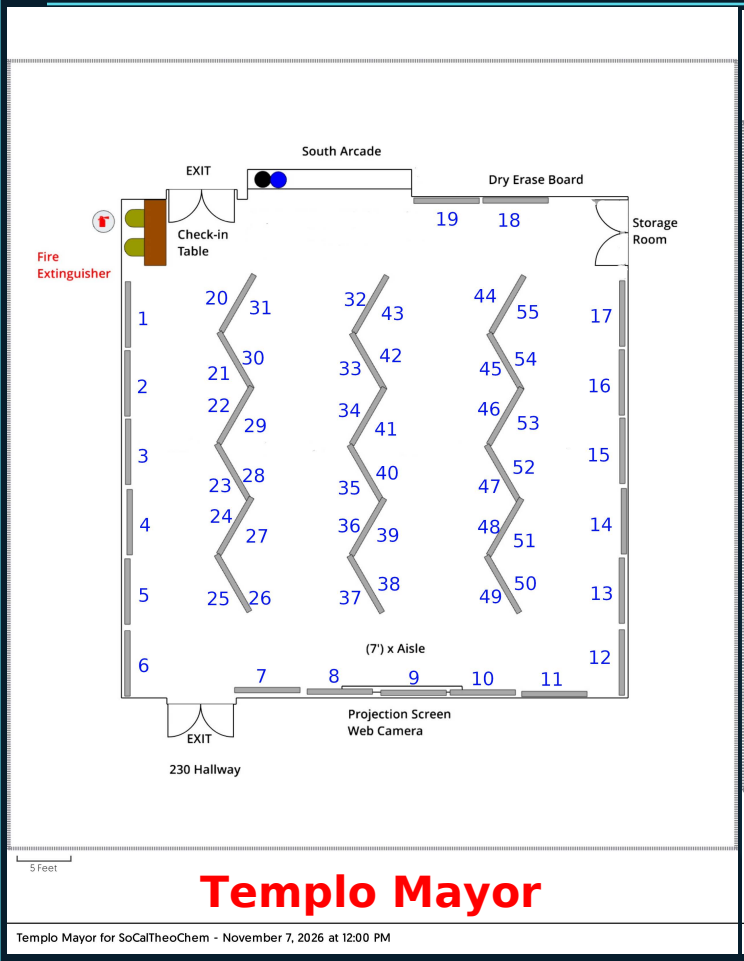
Saturday, November 7, 2026 | San Diego State University Student Union

| TIME | PROGRAM | LOCATION |
|---|---|---|
| 12:00-1:30 pm | Lunch | Union 3rd Floor |
| 12:30-2:00 pm | Poster session | Templo Mayor Mata'yuum |
| 2:00-2:10 pm | Symposium photo | Union 1st floor |
| 2:10-2:40 pm | **Negin Forouzesh, Cal State LA**: Physics-Informed Machine Learning for Drug Discovery: From Binding Free Energies to Molecular Design | Union Theater |
| 2:40-3:10 pm | **Ruqian Wu, UC Irvine:** Understanding chemical properties of nanostructures from DFT simulations | Union Theater |
| 3:10-3:40 pm | **Ryan Cammarota, Cal State Fullerton:** Molecular Descriptors and Data Science Tools for Scalable Reaction Outcome Prediction | Union Theater |
| 3:40-3:55 pm | Coffee break / poster break-down | Union 3rd Floor / Templo Mayor / Mata'yuum |
| 3:55-4:15 pm | **Mohammad Ahsan, UCLA:** From Motion to Mechanisms: Edge-Aware Graph Attention Networks for Interpretable Molecular Dynamics | Union Theater |
| 4:15-4:45 pm | **Kara Fong, Caltech:** Molecular Origins of Specific-Ion Effects in Electrocatalysis | Union Theater |
| 4:45-5:15 pm | **Thomas Fay, UCLA:** A Molecular Perspective on the Chirality Induced Spin Selectivity Effect | Union Theater |
| 5:15-5:20 pm | Poster awards; closing | Union Theater |

# Poster Session

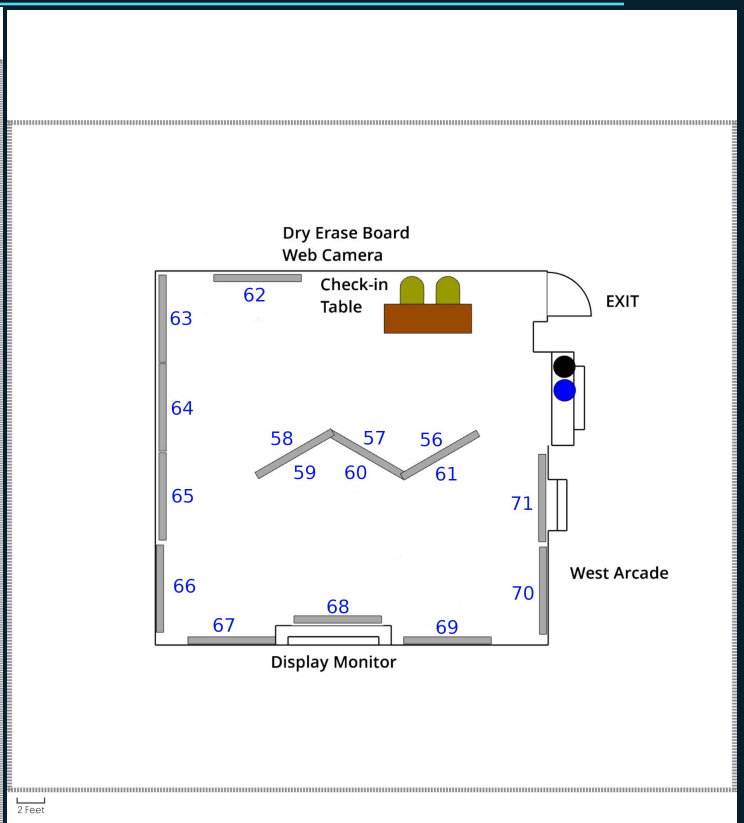
**12:30-2:00pm**

Templo Mayor and Mata'yuum, Aztec Student Union, 2nd floor




**Templo Mayor**

Templo Mayor for SoCalTheoChem - November 7, 2026 at 12:00 PM




**Mata'yuum**

Mata'yuum for SoCalTheoChem - November 7, 2026 at 12:00 PM

Presenters: we will have to tape posters 1-61 to the poster boards. If you can apply a strip of packing tape to the back of your poster at each corner before arriving, it will help installation go a little faster.

Posters 62-71 will be pinned to foamboard, so no need for tape on the back.

# Dining Near the Union

## OPTIONS FOR A MEAL BEFORE THE DRIVE HOME

If you are staying in the area after the symposium, these nearby options are convenient for dinner before heading back toward Los Angeles or Orange County.

### Oggi's Pizza

**SATURDAY: 12:00-8:00 PM**

**Union 1st floor**

Pizza, salads, wings, and casual group-friendly dining.

### Habit Burger Grill

**SATURDAY: 10:00 AM-10:00 PM**

**Union 1st floor**

Burgers, sandwiches, fries, and quick casual dining.

### Starbucks

**SATURDAY: 8:00 AM-10:00 PM**

**Union 1st floor**

Coffee, tea, pastries, and lighter food options.

### Eureka

**SATURDAY: 11:00 AM-MIDNIGHT**

**ACROSS THE BUSWAY |**

American food, craft drinks, and a sit-down dinner option.

Other options are available further south on College Ave and west along Montezuma Blvd.

# SoCal TheoChem 9
# ORAL SESSION ABSTRACTS

9:00-9:30am

*Correlated excitations across space and time: Electron-phonon interactions, Wigner crystalline excitons, and ultrafast nonequilibrium dynamics*

**Zhenglu Li, USC**

The past few years have seen rapid progress in understanding how correlations shape the excited states of materials. In this talk, I will present a unified first-principles framework enabled by recent advances in many-body perturbation theory to study correlated excitations and their coupling with phonons, both in and out of equilibrium. I will first discuss the critical role of electron-phonon coupling in correlated materials, introducing recent progress in GW perturbation theory [1] that uncovers self-energy-renormalized interactions in kagome superconductors [2-4], as well as previously overlooked many- body effects in long-range polar Frhlich coupling [5]. I will then show how strongly correlated excitons emerge from the generalized Wigner-crystal ground states in transition-metal dichalcogenide moir superlattices [6], using GW-Bethe-Salpeter equation calculations. Finally, I will present a time-dependent GW approach with coupling to phonons included across the full Brillouin zone [7], which captures the nonequilibrium and coherent exciton-phonon coupled dynamics, illustrated through pump-probe photoemission simulations of two-dimensional materials. These studies outline a comprehensive framework for studying correlation phenomena in energy and quantum materials from first principles.

[1] Phys. Rev. Lett. 122, 186402 (2019).
[2] Phys. Rev. Lett. 126, 146401 (2021).
[3] Phys. Rev. Lett. 133, 126401 (2024).
[4] Phys. Rev. Lett. 134, 106401 (2025).
[5] Phys. Rev. Lett. 137, 146401 (2026).
[6] Proc. Natl. Acad. Sci. 123, e2531259123 (2026).
[7] arXiv:2607.15411 (2026).

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9:30-10:00am

*Density Functional Theory: From the mundane to the outer limits*

**Kieron Burke, UC Irvine**

Density functional theory (DFT) is the workhorse of electronic-structure calculations, but even after six decades, there are endless things to discover. I will describe five works from this year, each championed by a brilliant young researcher, spanning a wide range of DFT and its applications. You will learn how to:

Predict accurate KohnSham densities with machine learning, enabling molecular dynamics with access to electronic properties.

Extract better energies in solid-state DFT calculations using HartreeFock densities, especially for molecular crystals.

Uncover electronic correlations in Kagome lattices using conditional-probability DFT.

Unite time-dependent DFT and ensemble DFT to describe electronic excitations.

Improve approximate DFT energies by deliberately using the wrong number of electrons!

With this smorgasbord, I hope there will be something of interest for everyone.

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10:20-10:50am

*Short-Range Order as a Design Variable for Complex Multielement Electrocatalysts*

**Wanlu Li, UC San Diego**

Multielement electrocatalysts offer a large compositional and structural space for tuning catalytic performance, but their chemical and structural disorder makes it challenging to identify the atomic environments that govern stability and reactivity. In this talk, I will introduce computational approaches that use short-range order (SRO) to model and design these complex materials. First, I will present ApolloX, a generative framework that combines SRO descriptors with a conditional machine-learning generative model and particle swarm optimization to explore the structures of disordered materials. Using amorphous FeCoNiMoBO as an example, I will discuss how boron modifies local metaloxygen and metalmetal coordination and influences amorphization and oxygen evolution performance. I will then introduce ARCADE, an automated workflow that connects multielement catalyst structures with adsorption energetics and catalytic properties. For LaSnBi-based high-entropy catalysts for formic acid formation, analysis of local chemical environments reveals how SRO relates to structural stability, activity, and selectivity. Together, these examples illustrate how SRO can serve as a design variable for connecting atomic structure to catalytic function.

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10:50-11:20am

*Computational astrochemistry from the spectroscopy and formation of PAHs to interstellar photochemistry*

**Vincent Esposito, Chapman University**

Newly developed computational methods now allow for the disentanglement of the CD and CN stretches of deuterated (D) and cyano (CN)-substituted polycyclic aromatic hydrocarbons (PAHs) in astronomical IR spectra from the James Webb Space Telescope. Gas-phase PAHs are ubiquitous forms of carbonaceous matter spread throughout the universe, and their emission, along with that of dust, is thought to dominate the near- and mid-IR spectrum of various astronomical sources such as protoplanetary disks, planetary nebulae, and galaxies. To better understand the nature of this emission, advanced anharmonic quantum chemical methods in concert with high-resolution experiments at the HFML-FELIX institute in The Netherlands have been used to explore the spectroscopic characteristics of D- and CN-PAHs. Additionally, new formation mechanisms are proposed for the production of cyanobenzene in the atmosphere of Titan, Saturns largest moon. Finally, excited state photochemistry reveals the (in)stability of small complex organic molecules in the harsh radiation fields of interstellar space and molecular clouds.

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11:20-11:40am

*Ensemble Time Dependent Density Functional Theory*

**Kimberly Daas, UCI**

Linear Response Time-Dependent Density Functional Theory (LRTDDFT) gives access to accurate transition frequencies and oscillator strengths of low-lying optical excitations. However, because LRTDDFT is based on small perturbations around the ground-state potential, it cannot describe transitions between excited states, crucial to explain, for example, pump-probe laser experiments. Recently, an alternative approach to obtain transition frequenciesEnsemble DFThas regained attention, which incorporates information about all eigenstates in its ensemble. By combining these methods, Ensemble TDDFT (ETDDFT) offers a variety of new cost-effective approaches to recover excited-state to excited-state transitions and double excitations that are beyond LRTDDFTs reach. In this talk, we present exact ensemble formulations of key equations, such as the Adiabatic Connection Fluctuation-Dissipation Theorem. These exact and approximate results are illustrated using the symmetric two-site Hubbard model at half-filling.

11:40am-12:00pm

*Tracking the Evolution of Electronic Character of Ground and Excited States with Mixed-Reference Spin-Flip TDDFT* (see also Poster 44)

**Arnab Chakraborty, USC**

Molecular torsion and increasing conjugation length can change the electronic character of ground and excited states, often introducing substantial multiconfigurational character. Describing these changes requires both an efficient electronic-structure method and analysis tools that go beyond excitation energies. Mixed-reference spin-flip time-dependent density functional theory (MRSF-TDDFT) extends the applicability of standard TDDFT to strongly correlated states while substantially reducing the spin contamination associated with original spin-flip TDDFT. We present an efficient implementation of MRSF-TDDFT in Q-Chem, providing excitation energies, oscillator strengths, spin-orbit couplings, and transition density matrices. Integration with libwfa enables density-based characterization using natural orbitals, natural transition orbitals, natural difference orbitals, and excitonic descriptors. We first examine how electronic character changes with molecular geometry, following the evolution of diradical character along torsion in tetramethyleneethane and examining the ground and first excited singlet states near a conical intersection in the retinal model PSB3. Comparisons with high-level wave function calculations assess the description of these states, while spin-orbit couplings in selected diradicals demonstrate the effectiveness of the approach. We then turn to two important families of conjugated systems, polyenes and polyacenes, to follow changes in single-excitation character and exciton descriptors in their low-lying valence states with increasing conjugation length. Together, these studies show how MRSF-TDDFT equipped with density-based analysis helps reliably interpret trends in state energies and spectroscopic properties and follow changes in electronic character as states mix and change order.

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2:10-2:40pm

*Physics-Informed Machine Learning for Drug Discovery: From Binding Free Energies to Molecular Design*

**Negin Forouzesh, Cal State LA**

Accurate prediction of proteinligand binding free energies and efficient exploration of chemical space are central challenges in computational drug discovery. Physics-based methods provide valuable descriptions of molecular interactions, while machine learning offers flexible representations and rapid predictions. Integrating these approaches requires careful consideration of how physical information guides model architecture, training, and molecular selection.

In this talk, I will present three related directions from our work on physics-informed machine learning. First, I will introduce neural networks that combine graph-based molecular representations with energetic features from implicit solvent calculations to predict binding free energies, with applications ranging from hostguest systems to proteinligand complexes. Second, I will discuss deep generative models coupled with physics-informed active learning, in which generated ligands are evaluated using docking and implicit solvent calculations, selected, and incorporated into iterative model refinement. This framework provides a way to guide molecular generation using computational feedback across different generative architectures. Finally, I will examine multi-objective optimization strategies for balancing agreement with experimental binding data and consistency with physics-based estimates, including methods that address conflicting gradients during training.

Together, these studies illustrate complementary ways to incorporate physical knowledge into molecular machine learning. I will discuss their computational performance, limitations, and implications for developing more reliable binding predictors and prioritizing candidate molecules for further investigation.

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2:40-3:10pm

*Understanding chemical properties of nanostructures from DFT simulations*

**Ruqian Wu, UC Irvine**

Nanostructures offer unique opportunities to tailor chemical properties through control of their size, composition, and atomic structure, with important applications in catalysis and energy conversion. Advances in computational methods and hardware have made density functional theory (DFT) a powerful tool for understanding and predicting their formation, stability, and chemical reactivity. In this talk, I will highlight several examples from our research, including the formation of PtCo coreshell nanoparticles, chemical reactions confined within scanning tunneling microscopy (STM) nanocavities, and CO capture and conversion. These studies illustrate how first-principles simulations reveal the atomic-scale mechanisms underlying chemical processes and establish connections between electronic structure, reaction pathways, and chemical functionality. Together, they demonstrate the potential of DFT to guide the rational design of nanomaterials for practical chemical applications.

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3:10-3:40pm

*Molecular Descriptors and Data Science Tools for Scalable Reaction Outcome Prediction*

**Ryan Cammarota, Cal State Fullerton**

The applications of machine learning (ML) and data science tools in the field of chemistry have risen meteorically over the past decade. However, training sophisticated ML algorithms (e.g., neural networks) to predict reaction outcomes requires a vast amount of experimental training data that is seldom available. The most common scenario encountered by chemists remains the desire to make reliable reaction predictions based on relatively small data sets (10 to 100 experimental observations). In this small data regime, learning the relationship between calculated molecular properties and experimental reaction outcomes is the prevailing approach. A key challenge remains the efficient translation of complex molecules into numerical inputs, known as molecular descriptors. My research groups core hypothesis is that designing more chemically meaningful descriptors will allow supervised learning algorithms to more precisely learn about underlying chemical phenomena, thereby enabling more generalizable predictions that extend further beyond a limited training set and into broader domains of substrate and reaction applicability. In this talk, our findings on the predictive utility of existing molecular descriptor classes will be compared across case studies of reported metal-catalyzed CH functionalization reactions, with the identified limitations of existing steric descriptors inspiring us to develop new designer descriptors. We have recently developed a dynamics-informed spatial molecular descriptor, Direct Approach Radial Trajectories (DARTs), which quantifies potential substrate approach paths within each quadrant of flexible catalyst reactive sites. DARTs descriptors have been shown to improve enantioselectivity predictions in dirhodium-catalyzed cyclopropanation reactions and may be generally useful for quantitative stereoselectivity prediction in other organic reactions. More broadly, this talk will emphasize how physically meaningful descriptors derived from relatively inexpensive computational methods can capture important factors driving reaction selectivity to provide scalable computational prediction platforms.

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3:55-4:15pm

*From Motion to Mechanisms: Edge-Aware Graph Attention Networks for Interpretable Molecular Dynamics* (see also Poster 39)

**Mohammad Ahsan, UCLA**

Molecular dynamics simulations generate extraordinarily rich descriptions of biomolecular motion, yet the interactions that actually organize these motions into folding, allostery, and assembly mechanisms are often buried within millions of correlated fluctuations. We developed an interpretable graph-attention framework that learns directly from MD trajectories and converts dynamical prediction into mechanistic insight. Biomolecules are represented as dynamic interaction graphs, and graph attention networks (GATs) are trained to predict how molecular configurations evolve in time. Rather than treating the learned attention as a black-box intermediate, we use it to identify interactions and residues that dominate dynamical information flow. Applied to CRISPR-associated TnsC filaments, this approach exposed early inter-subunit recognition events that precede productive filament elongation and revealed how the interaction network reorganizes as assembly progresses. We next asked whether explicitly encoding molecular physics into the graph edges could sharpen both prediction and interpretation. We therefore developed Edge-Conditioned, Edge-Injected, and Edge-Gated architectures that incorporate pairwise physical interaction features directly into attention and message passing. Across systems spanning protein folding, allosteric regulation, and large biomolecular assemblies, edge-aware models recover distinct layers of mechanism that are obscured by structure-only representations. In Chignolin, attention networks identify interactions associated with the folding; in HIV-1 protease, they resolve mutation-dependent rewiring between distal regions, the flaps, and the active site; and in TnsC assemblies, they capture interaction patterns associated with oligomerization and filament growth. These results suggest that graph attention can serve not only as a predictor of molecular motion, but as a microscope for interrogating it. By transforming MD trajectories into residue-level, physically grounded interaction networks, edge-aware GATs provide a general framework for discovering the molecular pathways that connect structure, dynamics, and function.

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4:15-4:45pm

*Molecular Origins of Specific-Ion Effects in Electrocatalysis*

**Kara Fong, Caltech**

Electrolytes influence electrochemical reaction rates and selectivities through coupled effects on interfacial structure, reaction energetics, and molecular transport. Disentangling these effects is essential for understanding and ultimately controlling electrochemical reactivity. We examine this problem in electrochemical nitrate reduction, where reaction rates depend strongly on the identity of the supporting electrolyte cation. Using classical molecular dynamics simulations in the constant-potential ensemble, we find only weak cation dependence in the free energy of nitrate adsorption. This behavior reflects the dominant role of water in shaping the interfacial potential profile and the suppression of nitrate-cation pairing near the electrode by image-charge effects. Instead, we find that bulk transport can reconcile the experimental trends: electrolytes with higher conductivity and lower nitrate transference numbers reduce the energetic penalty for transporting anionic nitrate toward the negatively polarized electrode, thereby enhancing nitrate delivery to the surface. These results offer a broader framework for understanding specific-ion effects in electrocatalysis by highlighting the role of macroscopic transport alongside interfacial phenomena. I will conclude by placing this study within our broader efforts to understand and control electrolyte effects across electrochemical interfaces and nanoconfined environments.

*References*

[1] Madeline A. Murphy and Kara D. Fong. "Beyond Interfacial Structure: Ion Transport Mediates Cation Effects in Electrochemical Nitrate Reduction." ACS Electrochemistry 2.4 (2026): 983-994.

4:45-5:15pm

*A Molecular Perspective on the Chirality Induced Spin Selectivity Effect*

**Thomas Fay, UCLA**

Much of the pioneering experimental and theoretical work the chirality induced spin selectivity effect has focussed on spin-dependent conductivity of chiral molecules between electrodes. Although instrumental in the development of our current understanding of the CISS effect, these set-ups are complicated by the interplay of effects arising from the chiral molecule directly and interactions with electrodes. Arguably a simpler set-up, which I will outline in this talk, is to consider photo-excitation induced electron transfer in chiral molecules, where the affect of chirality on electron transport can potentially be probed more directly. In particular I will describe a theory of how electron spin coherence[1] and spin polarization[2] can be generated in chiral molecular systems in the absence of electrode interfaces. These effects emerge in systems where charge transport is dominated by incoherent hopping, mediated by spinorbit and electronic exchange couplings. In this talk I will present the theory of these effects, and the general principles we can use to understand chirality induced spin effects in molecular systems. Furthermore, I will outline how chirality induced spin effects could be probed experimentally, and how it can also manifest in charge recombination reactions [3]. These ideas have also recently been employed to show that spin-polarization can lead to enantioselective chemical reactions [4]. Chirality induced spin coherence and polarization effects should appear in many chiral systems, and the ideas I will present have implications for general spin transport phenomena.

Publication: [1] Fay, T. P. Chirality-Induced Spin Coherence in Electron Transfer Reactions. J. Phys. Chem. Lett. 12, 14071412 (2021).
[2] Fay, T. P. & Limmer, D. T. Origin of Chirality Induced Spin Selectivity in Photoinduced Electron Transfer. Nano Lett. 21, 66966702 (2021).
[3] Fay, T. P. & Limmer, D. T. Spin selective charge recombination in chiral donorbridgeacceptor triads. J. Chem. Phys. 158 194101 (2023)
[4] Fay, T.P. Enantioselective radical reactions can be induced by electron spin polarization: A quantum mechanism for Nature's emergent homochirality? J. Phys. Chem. Lett. 16, 94149420 (2025)

# SoCal TheoChem 9
# POSTER ABSTRACTS

Poster 1:

*All-Atom Molecular Dynamics of Vibronic "Molecular Jackhammers" Disrupting Lipid Bilayers*

**Felicia Jin, Selene Chang, Timothy Mai, Praveen Prabhakar, Ioan Andricioaei**
University of California, Irvine (UCI)

Aminocyanine dyes such as Cy7.5 and Cy7 recently termed "molecular jackhammers" mechanically destroy cancer cell membranes when activated by near-infrared (NIR) light. Unlike photodynamic and photothermal therapies, this action does not depend on reactive oxygen species; instead, NIR excitation drives whole-molecule vibronic motion (coupled plasmon-phonon modes) that ruptures the bilayer. Atomistic detail into this mechanism is unknown, and the details into how these jackhammers latch onto the lipid membrane is not well understood. We use all-atom molecular dynamics (MD) to provide this insight. To accurately model the structures of Cy7.5 and Cy7, the two structures were parameterized for the CHARMM36/CGenFF force field using the Force Field Toolkit (FFTK), with partial charges, bonded terms, and torsional profiles derived from ORCA quantum-mechanical calculations. The optimized dye is embedded in a DPhPC bilayer solvated with explicit water and simulated with NAMD3. Because classical MD cannot reproduce plasmon-phonon coupling directly, we identify the longitudinal and axial normal modes by choosing the normal mode that best resembles it, and apply targeted biasing forces along it, tracking kinetic-energy transfer from the dye into the surrounding lipids. We aim to quantify changes made to the membrane by measuring the area per lipid, bilayer thickness, S_CD order parameters with the jackhammer embedded in the lipid without any biasing forces as a control. These simulations will reveal how vibronic actuation couples to and mechanically fails lipid bilayers.

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Poster 2:

*Emergent Chirality in Copper-Imidazole Complexes: Cu(II) Propeller Conformers and Cu(I) Helical Oligomers*

**Amirzhaikyzy, Perizat; Lam, David; Oaxaca, Leslye Shanery; Osegueda, Nicole A.; Zargaroff, Jasmine, Alvarez Marcos**
Los Angeles Mission College

Copper ions participate in electron transfer, metalloenzyme catalysis, and metal homeostasis, while the imidazole side chain of histidine is a common biological copper ligand. Motivated by these roles, we applied computational methods to compare compact and extended Cu(I)- and Cu(II)-imidazole candidates and to examine how oxidation state and nuclearity shape aggregation and chirality. Before moving to aqueous models, we calibrated our protocol against the experimental gas-phase Cu-imidazole dissociation energy (D = 287.5 kJ mol): B97X-D4/def2-TZVP gave approximately 300.0 kJ mol, whereas r2SCAN-3c overbound at approximately 323.4 kJ mol. Calculations were performed with ORCA. r2SCAN-3c served to screen geometries; selected structures were refined and frequency-validated with B97X-D4/def2-TZVP, def2/J, RIJCOSX, and CPCM(Water). GOAT conformer searches at GFN2-xTB/ALPB(Water) sampled alternative topologies. Cu(I) models included compact and extended structures, with exploration extending through CuIm. The smallest aggregation steps show that CuIm does not dimerize favorably and that CuIm is a plausible, though entropy-limited, growth motif (G +8.0 kJ mol for association of two CuIm units). As nuclearity increases, unconstrained chainlike starting structures twist into serpent-like helices. A CuIm serpent and CuIm, CuIm, and CuIm helices are frequency-validated minima. In matched isomer comparisons, the Cu serpent lies 18.3 kcal mol below a compact trigonal-bipyramidal isomer at r2SCAN-3c, and the high-level Cu serpent is favored over a compact pentagonal-bipyramidal-derived jewel by 31.5 kcal mol in Gibbs free energy. Cu(II) gives a distinct and surprising form of chirality. The aqueous [Cu(Im)] minimum retains a square-planar CuN core,

but its four imidazole rings tilt approximately 45–47 in the same rotational sense, producing a propeller arrangement with a non-superimposable mirror image. We therefore describe this as conformational or propeller chirality, potentially dynamic if Cu-N rotation enables racemization. Ongoing calculations are expanding Cu(II)-imidazole assemblies toward eight copper centers. Predicted low-energy targets will guide planned synthesis and isolation. Together, these results connect gas-phase method calibration with biologically relevant aqueous coordination and identify oxidation-state-dependent routes to chirality.

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Poster 3:

*E3AO - A general learning framework for predicting the Quantum Wavefunction of the Hydrated Electron*

**Lixing Zhang and Benjamin Schwartz**

UCLA

Predicting the properties of the hydrated electron ($e^-_{\mathrm{hyd}}$) is challenging, as its diffuse wavefunction is very sensitively to fluctuations in the surrounding solvent. Such coupled responses directly characterize $e^-_{\mathrm{hyd}}$'s structure, dynamics, and reactivity. Molecular dynamics based on density functional theory (DFT) provides ab initio access to wavefunction evolution but is limited to small systems and short trajectories by its high computational cost. Machine-learned force fields (MLFFs) have emerged as promising alternatives because of their substantially lower cost. However, most MLFFs propagate only the solvent nuclei and omit electronic information essential to hydrated-electron chemistry. Here, we introduce E3AO, an equivariant neural network that efficiently predicts electron wavefunctions from instantaneous solvent configurations. At negligible cost relative to DFT, E3AO achieves 99.9% wavefunction fidelity on validation dataset and accurately captures the electrons position, spatial shape, and dynamical correlations. Moreover, E3AO learns a compact, data-efficient wavefunction representation that generalizes beyond interpolation, enabling few-shot transfer to substantially larger systems and characterization of hydrated-electron formation following non-equilibrium electron injection. The framework established here can be readily extended to charge-density prediction in broader settings and provides a foundation for future electron-aware neural-network force fields.

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Poster 4:

*Exploring Computational Workflows for Accurate and Efficient Prediction of Rotational Barriers between Atropisomers*

**Nilay Kanova Dogan, Jae Yoon Lee, Yuezhi Mao**

San Diego State University

Atropisomerism refers to axial chirality arising from hindered rotations around -bonds and plays an increasingly important role in medicinal chemistry, as many recently FDA-approved drugs contain atropisomeric axes. The rotational barrier between atropisomers is a key parameter that determines whether atropisomers remain conformationally stable or undergo rapid interconversion. In this work, we benchmarked computational workflows for predicting rotational barriers across three related molecular series with varying substituent groups: 3-aryl indoles, cyclopropanated intermediates formed upon carbene addition, and 4-aryl quinolines. These species correspond to the reactants, intermediates, and products of a Rh(II)-catalyzed atropisomer-selective ring expansion and exhibit low, medium, and high rotational barriers. As a first step, we obtained reference rotational free energy barriers (G) through rigorous transition-state optimization using density functional theory (DFT) and established that the energy barriers (E) closely approximate the computationally more demanding G values. Using E for subsequent benchmarking, we examined the accuracy of relaxed dihedral scan with DFT, a commonly used workflow for calculating rotational barriers, and obtained mean absolute percentage errors (MAPE) of 13.1%, 1.6%, and 6.3% for the indoles, cyclopropanated intermediates, and quinolines, respectively.

We then investigated how lower-cost methods, such as GFN-FF (a force field), GFN2-xTB (a semi-empirical quantum mechanical method), and UMA (a recently developed machine-learning potential), can contribute to efficient workflows for atropisomer rotational barrier prediction. Our results show that direct estimation of barriers from the highest-energy points on the geodesic paths connecting two atropisomers generated using UMA yields MAPE of 15–25% across the three molecular series, which may not be sufficient for quantitative prediction. However, we found that the highest-energy points along paths generated using these lower-cost methods provide reliable starting structures for subsequent DFT transition-state optimizations, which is more efficient than conventional approaches for generating transition-state guesses such as the nudge elastic band method or DFT-based relaxed dihedral scans. Overall, our benchmark provides practical guidance for accurate and efficient prediction of rotational barriers between atropisomers using state-of-the-art computational methods.

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Poster 5:

*Mechanism of Indium-Catalyzed copolymerization of Lactide and Caprolactone: A Theoretical Approach*

**Michael Pung, Kritika Sharma, Hootan Roshandel, Parisa Mehrkhodavandi, Paula L. Diaconescu**

University of California, Los Angeles

We present calculations for the block copolymerization system of lactide and caprolactone by a dinuclear indium catalyst. Prior experimental studies have shown that while lactide is polymerized by a monoalkoxy dinuclear indium species, caprolactone is instead polymerized by a bisalkoxy dinuclear indium species instead. Density functional theory calculations reveal that the active catalyst for caprolactone polymerization is a different conformer than the proposed catalyst observed by nuclear magnetic resonance spectroscopy. Further, calculations have shown that both alkoxides can act as intiators which is consistent with experimentally-determined molecular weights from size-exclusion chromatography.

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Poster 6:

*High-Q microresonators harvest quantum rare events*

**Sricharan Raghavan Chitra, Arghadip Koner and Joel Yuen-Zhou**

University of California San Diego

Classical linear optics posits that at sufficiently low intensities, light propagation in dielectric media is governed solely by their linear susceptibilities. Here, we demonstrate a departure from this paradigm in high-quality (high-Q) microresonators, where prolonged photon confinement enables rare quantum electrodynamical (QED) events, mediated by the quantum vacuum, to embed distinctive Raman signatures of the coupled analyte into the resonators linear transmission spectrum despite their absence from linear susceptibility. We further show that increasing the amount of adsorbed analyte sample amplifies these Raman fingerprints well above typical noise floors, rendering them experimentally accessible with state-of-the-art photonic architectures and detection schemes. This weak-coupling cavity QED effect offers unique routes to harness extended photon lifetimes and constrained geometries for leveraging vacuum fluctuations in next-generation photonic technologies for chemical and biological sensing and high-precision optical spectroscopy.

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Poster 7:

*Symmetry Restoration in the Hubbard-Holstein Model with Multireference Lang-Firsov States*

**Chenxi Wang and Zhihao Cui**

University of California, Irvine

Variational Lang-Firsov (LF) references offer a compact description of electron-phonon coupling, but their optimization can break the symmetries of finite Hubbard-Holstein systems. Near competing reference states, single-reference perturbative corrections may leave substantial energy errors. We develop

a variational multireference LF approach that combines symmetry-related, conditional coherent-state frames by solving a nonorthogonal configuration-interaction problem. For a four-site, one-electron ring, an eight-frame expansion reduces the LF-HF energy error near the localization crossover from 0.1092 to 0.00494 in units of the hopping amplitude. Adding selected frames improves the energy further. We next examine a four-site, four-electron ring, where our LF-HF benchmarks exhibit staggered spin density at weak electron-phonon coupling and charge order at stronger coupling. Even at zero electron-phonon coupling, LF-MP2 remains 0.2725 above exact electronic diagonalization for an on-site repulsion of four hopping units. We are extending the coherent-state frame construction to fixed multielectron determinant sectors and will compare symmetry, energies, and frame-space convergence with cutoff-converged exact diagonalization. This will test when mixing broken-symmetry LF references improves upon a single-reference treatment.

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Poster 8:

*WOX-WSe2 Heterostructures: A Pathway Toward Reliable Electrical Contacts*

**Jaedan Ford and Santosh KC**

SDSU

The introduction of two-dimensional (2D) materials such as transition metal dichalcogenides (TMDs) have become a crucial component of materials science and electronic device research. TMDs are composed of formula MX2, where M represents a transition metal (e.g. Mo or W) and X represents a chalcogen atom (e.g. S or Se), demonstrate high hole carrier mobility and large on/off ratios. However, the dangling free bond of TMDs limits their applications in electronic circuits as the contact resistance increases due to the van der Waals (vdW) forces at play between these layers. Recent research has utilized tungsten-oxide (WO3) as an intermediary layer between the TMD and the metallic layer to lower contact resistance and improve gate performance. This paper focuses on the interactions between tungsten-oxide and tungsten oxide with oxygen vacancy to investigate the underlying effects for the improved performance of the heterostructure. Due to the abundance of constituent elements and the scalability of 2D material synthesis, WOX-WSe2 heterostructures offer a sustainable and cost-effective solution to the next generation of electronic circuitry.

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Poster 9:

*Catalytic Activity of ZrO2 on Cu Inverse Catalyst Ensemble for CO2 Hydrogenation to Methanol*

**Zihan Yang, Anastassia N. Alexandrova, Philippe Sautet**

UCLA

The significant increase in CO2 emissions from heavy fossil fuel utilization has raised serious concerns, highlighting the need for effective methods to convert CO2 into value-added chemicals. Inverse ZrO2/Cu catalysts, where Zr oxide is deposited on Cu particles, show a high catalytic performance converting CO2 to methanol. A computational investigation on the catalytic activity of ZrO2 on Cu inverse catalysts for CO2 hydrogenation to methanol, considering highly dispersed ZrO2 trimers on Cu (111). Such clusters present a large ensemble of formate containing configurations, Zr3On(OH)m(OCHO)l, making the evaluation of the catalytic activity very challenging. We found that the sites on the various catalyst configurations exhibit markedly different activities for formate hydrogenation, despite their similar free energy and composition. To understand these differences in reactivity, we examined the structural and electronic nature of the low free energy catalyst configurations and identified that the energy of the lowest unoccupied orbital of the reacting formate, modified by its binding with the catalytic site, is a descriptor for the reaction energy of the formate hydrogenation step. From there, we screened an ensemble of catalyst structure using this descriptor to predict highly active metastable catalyst configurations. While conventional Cu/ZrO systems often exhibit the rate determining step at the formate hydrogenation, mechanistic information for inverse ZrO/Cu catalysts has been conflicting.

So, we also investigate the CO hydrogenation reaction mechanisms on a model of highly dispersed Zr oxide clusters on Cu (111). The exploration is not performed on a single active site configuration but across an ensemble of 83 formate configurations accessible under reaction conditions. Detailed reaction-pathway analysis reveals that structural sensitivity is pronounced, and only 10 of the catalyst configurations are significantly active across the full pathway. The turnover frequency of the studied inverse structures is largely determined by reaction steps after methoxy formation, rather than the formate hydrogenation steps, and the energy of the methoxy intermediate is a key reactivity descriptor. The reactivity is favored by partially reduced Zr clusters, and a Zr active site at an optimum distance from the Cu surface, close enough to provide hydrogen from Cu but not excessively close so as to overstabilize the methoxy reaction intermediate. Two hypotheses are presented for the ensemble average activity: where the probabilities of site populations are determined at the formate intermediate, or at the methoxy resting state. The latter, compared to the former, drastically changes the site distribution, eliminating active structures and decreasing the average rate by a factor 1000. Catalyst rigidity helps maintain activity by increasing isomerization barriers and slowing down the structural evolution from the more active formate-bound states to the less active methoxy-bound states. The approach therefore provides a microscopic view for one catalyst deactivation mechanism, and the two hypotheses appear to represent the different stages of the catalyst life cycle. Finally, simulated vibrational spectra under reaction conditions show excellent agreement with experimental DRIFTS measurements, providing further support for the proposed structures and mechanism.

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Poster 10:

*Unraveling the Role of Pendant Anionic Substituents in Tuning the Redox Properties of Ruthenium-Based Water Oxidation Catalysts*

**Nilay Kanova Dogan, Yuezhi Mao**

San Diego State University

Water oxidation catalysts based on ruthenium polypyridyl complexes provide highly tunable platforms for investigating how ligand structure influences redox behavior and catalytic performance. In this work, we employed density functional theory (DFT) calculations to examine the effect of pendant anionic substituents on the redox properties of a series of ruthenium complexes containing terpyridine and substituted phenanthroline ligands of the form [Ru(terpy)(phenX)], where X=SO3- ,COO- , andPO3iPr-. To quantify how through-space noncovalent interactions between these substituents and the ruthenium center affect redox properties, we first analyzed the RuII/III oxidation in a series of MeCN-bound surrogate complexes, in which the coordinating acetonitrile spatially separates the anionic groups and the Ru center and eliminates complications associated with proton transfer and further oxidation beyond RuIII. The results show that introducing pendant anionic substituents consistently lowers the RuII/III oxidation potential for the MeCN-bound complexes, indicating that these groups effectively modulate redox potentials through long-range electrostatic interactions as further confirmed by energy decomposition analysis and electrostatic potential calculations. We then extended the computational investigation to the corresponding aqua complexes, focusing on the proton-coupled oxidation of [RuII(terpy)(phenX)(H2O)] to form [RuIII(terpy)(phenX)(OH)], as well as the RuIV/V oxidation in the corresponding oxo-bound complexes. In contrast to the MeCN-bound surrogate complexes, the substituent-dependent trends are not fully preserved, as the oxidation energetics are influenced by additional factors such as proton transfer and structural rearrangement across oxidation states. These findings provide molecular-level insights into how second-sphere anionic substituents influence the redox properties of ruthenium-based water oxidation catalysts, demonstrating both the effectiveness and limitations of electrostatic tuning strategies.

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Poster 11:

*Representation-Invariant Subspace Formulation of Conical Intersection Search*

**Amogh Tundlam, Filipp Furche**

UC Irvine

Conical intersections (CIs) are fundamental funnels for non-radiative transition between electronic states, mediating the non-adiabatic dynamics of a vast array of photochemical processes. Despite their significance, the characterization of CIs within standard linear response time-dependent density functional theory (TDDFT) is often plagued by numerical instabilities and poor convergence. These challenges primarily arise from tracking individual states in the adiabatic basis in regions of degeneracy precisely where the Born-Oppenheimer approximation breaks down. Many current implementations of CI optimization rely solely on gradient differences and forego non-adiabatic couplings, offering a poor description of the CI branching space. Such implementations struggle to converge to the minimum energy crossing point of the CI as a result. To circumvent these issues, the TDDFT eigenvalue problem is instead reformulated as a stationary matrix Lagrangian over the entire subspace spanned by the relevant electronic states. Both the exact gradient and non-adiabatic coupling information of these states are encoded directly in the coordinate derivative of the stationary subspace matrix and are expressed in terms of representation-invariant matrix functionals. It is shown using degenerate perturbation theory that the first-order energy splitting away from the CI depends directly on the traceless part of the subspace matrix. This allows the characterization and optimization of CIs considering the subspace as a whole without relying on the adiabatic representation and explicit state tracking. This subspace-based framework offers a computationally efficient and numerically robust methodology for the characterization of excited state CIs and the systematic investigation of photochemical reaction mechanisms.

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Poster 12:

*Ultrafast nonlinear spectroscopy of polaritons: Semiclassical vs. quantum treatment*

**Michael Reitz, Joel Yuen-Zhou**

UCSD

We have recently introduced a general semiclassical framework for modeling the ultrafast nonlinear spectroscopy of molecular polaritons in the collective regime, based on a perturbative expansion of the coupled light-matter dynamics in the amplitudes and phases of the incident fields. This approach has enabled the efficient calculation and interpretation of pump-probe spectra, spatially resolved polariton transport, and multidimensional single- and double-quantum spectra, and can be combined with full-wave electrodynamics to treat realistic nanophotonic environments. Here, we investigate the connection between this semiclassical description and a fully quantum treatment based on the Tavis-Cummings model. By projecting the quantum density matrix onto excitation manifolds and constructing the perturbative hierarchy order by order, we identify how the larger set of quantum populations and coherences maps onto the reduced set of semiclassical light and matter variables. We show how these beyond-mean-field contributions enter nonlinear observables such as differential transmission, providing a route toward identifying spectroscopic signatures that distinguish genuinely quantum correlations in ultrafast experiments.

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Poster 13:

*Excited state photochemistry of hydroxylamine (NH2OH).*

**Juliana F. Jordan and Vincent J. Esposito**

Chapman

Photodissociation of gas-phase hydroxylamine (NH2OH) is most likely to occur along the N-O bond via non-adiabatic processes. NH2OH is a key component of primordial RNA in the RNA world hypothesis,

and its recent detection in the interstellar medium confirmed its presence in early space. Studies have been conducted on the formation of NH2OH on the surface of ices and subsequent diffusion into the gaseous state; however, few studies have examined its excited state photochemistry. In this work, the one-dimensional adiabatic potential energy surfaces (PESs) along each bond coordinate are computed using high-level multireference quantum chemical methods. Using these PESs, possible photodissociation routes are explored.

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Poster 14:

*An Ion-Neutral Reaction to Form Cyanobenzene and Ethynyl Benzene in Titans Atmosphere*

**Dr. Rachel Huchmala and Prof. Vincent Esposito**

Chapman University

The James Webb Space Telescope (JWST) continues to return high-resolution infrared (IR) spectra that are changing our understanding of the Universe. These spectra are riddled with features that are attributed to the polycyclic aromatic hydrocarbon (PAH) family of molecules. However, the formation of these molecules in space is an open question. This work capitalizes on anharmonic quantum chemistry calculations to explore reactions of the phenyl anion ($C_6H_5^-$) with cyano-substituted hydrocarbons that are present in Titans atmosphere. These new pathways and their associated energetics and kinetics provide insight into the formation of cyanobenzene through radical, anionic, and catalyzed reactions. In addition to developing an understanding of which cyano-substituted hydrocarbons and PAHs exist in space, accurate IR spectroscopic reference data are needed to aid in the search for them with JWST. To this end, a series of density functional theory (DFT) calculations have been conducted on the intermediates of the aforementioned reaction pathway and a series of cyano-PAHs to provide a computational benchmark for laboratory characterizations and observational searches of such molecules.

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Poster 15:

*Photodetachment Spectrum of Ring-Opened Oxirane Anion: A Computational Study*

**Bibhas Borah, Carson Baker, Debojyoti Dey, Nitai Sahoo, Anna I. Krylov**

University of Southern California

Ring-opened oxirane anions are believed to form during the photofragmentation of 3-oxetanone. Motivated by recent experiments in Professor Robert Continettis group, we investigated electronic structure of two possible isomers, CHCHO (CCO) and CHOCH (COC), and simulated their photodetachment spectra using high-level electronic structure methods from the Coupled-Cluster and Equation-of-Motion Coupled-Cluster (EOM-CC) family. The spectra were simulated using double-harmonic parallel-mode approximation. The neutral species produced by photodetachment feature complicated open-shell character and multiple electronic states. This poster will present the results of the calculations elucidating electronic structure of these species and discuss the comparison between the computed and experimental spectra.

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Poster 16:

*Real-Time Approach to the Dynamical Bethe-Salpeter Equation for Finite Systems*

**Tucker Allen, Barry Y. Li, Daniel Neuhauser**

UCLA

The GW-Bethe-Salpeter equation (GW-BSE) approach is an increasingly popular alternative to time-dependent density-functional theory (TDDFT) for molecular excited states, providing a more balanced treatment of excitations and improved accuracy for challenging Rydberg and charge-transfer states. However, standard implementations of GW-BSE employ static screening of the electron-hole interaction because treating its full frequency dependence is computationally demanding. We present a real-time linear-response approach to solving the dynamical BSE. The polarization part of the screened interaction

is obtained from time-dependent Hartree propagation of the one-particle density matrix within an orbital basis-set representation. The frequency convolution defining the dynamical kernel is evaluated as a product in time, avoiding numerical integration and storage of the full screened Coulomb operator. The resulting nonlinear eigenvalue problem is then solved directly. We benchmark the method on a set of small molecules and find small dynamical corrections for Rydberg excitations but larger corrections for n-to-$\pi*$ and $\pi$-to-$\pi*$ excitations. While the deterministic scaling remains O($N^6$), the time-propagation formulation is readily compatible with grid-based stochastic sampling methods, opening the possibility of dynamical BSE calculations for much larger molecular systems.

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Poster 17:

*Developing Machine Learning Interatomic Potential to Study CO2 Dynamics under Applied Potential*

**Madeline Murphy, Kara Fong**

California Institute of Technology

Molecular dynamics (MD) simulations are widely used to study ion transport in electrolytes and electric double layer (EDL) structure at electrode/electrolyte interfaces. Classical force fields, though computationally tractable, lack the accuracy needed to resolve these properties, while ab initio methods are too costly to simulate the relevant time and length scales. Machine learning interatomic potentials (MLIPs) offer near-ab initio accuracy at much lower cost by learning the potential energy surface from atomic coordinates. In this work, we train a short-range MACE model on DFT data for aqueous KHCO and use it to compute concentration-dependent transport coefficients via GreenKubo relations. The MLIP gives better agreement with experimental conductivity than an empirical force field, a difference we trace to weaker cationanion correlations. However, short-range MLIPs cannot capture long-range electrostatics, which are integral to electrode/electrolyte interfaces. We assess three approaches to incorporate long-range interactions: latent charges (MACE-LES), global charge equilibration (MACE-Polar), and a hybrid approach that overlays classical Coulomb interactions with fixed partial charges on a short-range MACE model trained on the DFT residual. Charge-induction tests at a Cu/water interface show that the latent-charge model responds poorly to changes in electrolyte charge, while charge equilibration spuriously distributes excess charge onto water molecules. In contrast, the hybrid model reproduces bulk water structure and correctly captures interfacial water dipole alignment and dielectric screening without compromising short-range accuracy. This framework will be used to study the behavior of CO in the EDL, including its adsorption free energy, transport through the diffuse layer, and solvent response to step changes in potential.

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Poster 18:

*Anharmonic Vibrational Spectroscopy of Functionalized Benzenes*

**Megan Kim and Dr. Vincent J. Esposito**

Chapman University

Anharmonic vibrational frequency computations using density functional theory produced infrared (IR) spectra within 2% of the experimental data for various substituted benzene molecules. Benzene and three of its derivatives (cyanobenzene ($C_6H_5CN$), ethynylbenzene ($C_6H_5C_2H$), and cyclohexadiene-1-thione ($C_6H_6S$)) have been detected within the interstellar medium (ISM). The James Webb Space Telescope (JWST) is providing high-resolution IR observations of astronomical sources such as galaxies, planetary nebulae, and protoplanetary disks. Recently, signatures of substituted aromatic molecules have being seen in JWST spectra. As a result, two methods are used to compute the IR spectra of functionalized benzenes. Comparison to experimental spectra from the literature shows high accuracy, often within 2% of the experimental data. These results indicate that the methods utilized here can be used to compute accurate vibrational spectra of larger substituted polycyclic aromatic hydrocarbons (PAHs).

Poster 19:

*Ultrafast Proton Transfer and Zundel-like Cation Formation in Ionized Liquid 1-Propanol*

**Haowei Wu, Taekeun Yoon, Debadarshini Mishra, Lars Hoffmann, Ramesh Jarupula, Martin Gral, Christina Y. Hampton, Surjendu Bhattacharyya, Martin Centurion, Xinxin Cheng, Daniel P. DePonte, Samuel W. Eisenberg, R. Joel England, Lauren F. Heald, Jun Heo, Doyeong Kim, Cheolhee Yang, Haeyun Jeong, Hyotcherl Ihee, Matthias Ihme, Fuhao Ji, Brian Kaufman, Matthias F. Kling, Jake D. Koralek, Randy A. Lemons, Melody Li, Mianzhen Mo, Krishna Murari, J. Pedro F. Nunes, Samuel Sahel-Schackis, Stephen P. Weathersby, Tianzhe Xu, Ming-Fu Lin, Patrick Kramer, Oliver Gessner, Wan-Lu Li, Yuezhi Mao, Alexander Reid, Yusong Liu, Haiwang Yong**

UCSD

Tracking proton transfer in ionized liquids in space and time remains challenging because it is coupled to rapid rearrangements of the surrounding hydrogen-bond network. Here, we combine megaelectronvolt ultrafast electron diffraction with ab initio molecular dynamics simulations to investigate the femtosecond structural dynamics of neat liquid 1-propanol following multiphoton ionization. The experimental diffraction signals and simulations reveal an initial intermolecular proton transfer accompanied by transient hydrogen-bond strengthening, followed by the formation of Zundel-like cations, where a proton is dynamically shared by two 1-propanol molecules. The findings are validated with the double-well free energy profile. Time-dependent radial distribution functions extracted from the non-equilibrium simulations connect the structural changes to the measured diffraction signals. These results extend the observation of transient Zundel-like configurations beyond aqueous systems to a liquid alcohol, where alkyl groups constrain the connectivity of the hydrogen-bond network. This work provides a structural picture of how photoionization initiates proton transfer and generates reactive ionic species in liquid 1-propanol, with implications for understanding photochemical processes in organic liquid environments.

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Poster 20:

*Molecular Origins of Lithium-Ion Transport in the Anionic Metal-Organic Framework SU-102*

**Youhan Lu, Suman Saha, Vibhu Vardhan Singh, Zhentao Yang, Julius J. Oppenheim, Mircea Dinca, Francesco Paesani**

University of California, San Diego

Metal–organic framework (MOF) quasi-solid electrolytes offer chemically tunable environments for ion transport, but the molecular roles of framework coordination and confined solvent remain unclear. Here, we combined solid-state nuclear magnetic resonance (ssNMR) measurements with molecular dynamics simulations to determine the Li+ transport mechanism in propylene carbonate-filled SU-102. Variable-temperature direct- and cross-polarization Li7 ssNMR reveal two distinct Li+ populations with different local tumbling dynamics. Our simulations identified Zr-associated, linker-associated, and fully PC-solvated Li+ coordination environments. We found that Zr-associated sites provide the strongest thermodynamic stabilization, whereas the site-persistence function decays more rapidly for linker-associated Li+ over the simulated interval. The linker-associated state exhibits the largest trial-weighted displacement, and linker-to-linker hopping is the most frequent classified event under the sampled fields, followed by Zr-to-Zr hopping. Chemical color-diffusion nonequilibrium molecular dynamics yielded an ionic conductivity of 1.340.48 mScm-1 along the one-dimensional channels and a negligible conductivity perpendicular to them, corresponding to an orientationally averaged conductivity of 0.450.16 mScm-1, in close agreement with the experimental value of 0.52 mScm-1. Together, our results support a picture in which PC-assisted hopping between linker sites contributes more strongly than vehicular diffusion of fully solvated ions under the simulated conditions. We find that the most strongly stabilizing Li+ site is not necessarily the site that carries transport: Zr-node sites bind Li+

most strongly but form a discontinuous network along the pore axis, whereas the weaker-binding linker sites form a continuous one and dominate the sampled hopping statistics. Confined PC is retained in the coordination shell across these transfers rather than acting as a vehicle. These findings identify the balance between ion-framework stabilization and facile site-to-site exchange as a key design principle for reticular quasi-solid electrolytes.

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Poster 21:

*Predictive Biochemical Simulations from First Principles*

**Chenghan Li and Garnet K.-L. Chan**

UC Irvine

Predicting enzyme reaction mechanisms from first principles requires methods that can describe both strongly correlated reaction electrons and the statistical fluctuations of the surrounding protein.

I will present a data-driven strategy that connects high-accuracy quantum chemistry to enzyme-scale simulations. First, I will show a new coupled-cluster approach that significantly improves its accuracy in strongly correlated regimes, including bond dissociation and iron-sulfur clusters. Then I will briefly mention numerical methods to substantially accelerate coupled-cluster calculations with well-controlled errors.

These advances allowed us to reach the picosecond timescale in ab initio molecular dynamics on a CCSD(T) potential surface. I will show strategies to further extend simulations to biochemically relevant timescales through a hierarchical machine learning of quantum Hamiltonians. As an application, simulations of chorismate mutase yield a predicted reaction rate close to experiment without fitting to any experimental data.

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Poster 22:

*Excitation-energy regularization of perturbative triples for metallic coupled-cluster theory*

**Ruiheng Song, Hong-Zhou Ye**

UC Irvine

Coupled-cluster theory with single, double, and perturbative triple excitations [CCSD(T)] is highly accurate for molecules and insulating solids, but its perturbative triples correction diverges for metals in the thermodynamic limit. We introduce two dressed triples corrections that suppress the unscreened long-wavelength interaction while retaining the formal $\mathrm{O}(N^7)$ scaling and contraction structure of conventional (T). In both corrections, only the interaction that defines the approximate triples amplitudes is dressed, while the interaction that couples these amplitudes to the energy remains bare. The first uses the short-range component of a range-separated Coulomb interaction, denoted (srT), whereas the second uses an excitation-energy-dependent $\sigma$ regularizer, denoted ($\sigma$T). Both damping functions supply an additional factor proportional to $q^2$ at small momentum transfer, canceling the $q^{-2}$ Coulomb singularity at the dressed vertex and thereby removing the logarithmic infrared divergence of the triples energy. For the three-dimensional uniform electron gas, ($\sigma$T) exhibits substantially weaker density dependence than (srT): a single dimensionless coefficient gives CCD($\sigma$T) correlation energies within approximately 0.3 m$E_\mathrm{h}$ per electron of the diffusion Monte Carlo reference over $r_s = 1$–5. Transferring the same coefficient without further adjustment to body-centered-cubic lithium gives a CCSD($\sigma$T) cohesive energy of 59.8 m$E_\mathrm{h}$/atom, close to diffusion Monte Carlo and the zero-point-corrected experimental estimate. These results establish excitation-dependent dressing as a simple, minimally invasive regularization of perturbative triples for nearly-free-electron metals.

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Poster 23:

*Chiral molecular orbitals: a tool for visualizing chiroptical properties*

**Victoria Nazarova and Anna Krylov**

University of Southern California

Electronic circular dichroism (ECD) is a sensitive spectroscopic probe of molecular chirality, measuring the difference in absorption of left- and right-circularly polarized light. However, interpretation of ECD in terms of molecular-orbital contributions is not straightforward. Here, we introduce chiral molecular orbitals (chiral MOs), a new tool for providing an orbital-based description of ECD. Chiral MOs are obtained by decomposing the ECD cross sections into molecular-orbital contributions and visualized as real-space isosurfaces, offering an intuitive picture that links electronic structure to the optical response of the chiral molecule. Following the previous studies that implemented chiral MOs within TDDFT, we extend the theory to EOM-CCSD, both in the valence and in the core-level domains. We apply this tool to selected organic molecules. Our results demonstrate that chiral MOs directly connect molecular orbitals to the observed chiroptical response and provide a framework for understanding the electronic origin of chirality and related effects.

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Poster 24:

*Characterization of metastable electron-attached states of p-bromothiophenol*

**Debojyoti Dey and Anna I. Krylov**

University of Southern California

When an electron collides with a molecule, it can be scattered, excite the molecule, or attach to it. In closed-shell molecules that do not form stable anions, electron attachment often produces short-lived anionic states called resonances. Resonances play a central role in processes as diverse as DNA radiolysis, plasmonic catalysis, and attosecond spectroscopy.[1] These collision processes can be studied using electron energy-loss spectroscopy (EELS) in which electrons with a known energy collide with neutral molecules and their energy loss is measured. Electron scattering via resonances may lead to dissociative electron attachment (DEA) in which electron attachment causes a chemical bond to break. The theoretical description of resonances is challenging because these states belong to the continuum and have wavefunctions that are not $L^2$-integrable. The complex absorbing potential (CAP) approach, based on non-Hermitian quantum mechanics, provides a way to overcome this difficulty. In this approach, a purely imaginary absorbing potential is added to the Hamiltonian. Combining CAP with equation-of-motion coupled-cluster (EOM-CC) theory allows one to compute resonances as states with $L^2$-integrable wavefunctions and complex energies.[1] The real and imaginary parts of the energy provide the resonance position and width (the width determines the resonance lifetime). Our group has successfully applied this approach to interpret EELS experiments. [2,3] In this work, we use CAP calculations to identify the resonant states formed by electron attachment to p-bromothiophenol. This molecule is interesting because it has two possible dissociation pathways involving C-Br or S-H bond cleavage. We calculate the resonance positions and widths and use Dyson orbitals to determine the character of each resonance. We then investigate whether DEA occurs and which bond-cleavage pathway is favored.

References: [1] T. C. Jagau, K. B. Bravaya, and A. I. Krylov, Annu. Rev. Phys. Chem. 68, 525 (2017). [2] M. Mukherjee, T. P. Ragesh Kumar, M. M. Rankovi, P. Nag, J. Fedor, and A. I. Krylov, J. Chem. Phys. 157, 204305 (2022). [3] M. Mukherjee, C. Baker, M. M. Rankovi, P. Nag, J. Fedor, and A. I. Krylov, J. Chem. Phys. 163, 024120 (2025).

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Poster 25:

*How does BF3 Alter the Excited-State Behavior and Photoacidity of 2-Naphthols?*

**Destiny Heang, Keerthy P. Sudhakarian Nair, Dr. Andrew S. Petit, Dr. Jahan Dawlaty**
Cal State Fullerton

Photoacids are molecules that exhibit increased acidity upon electronic excitation, allowing them to release protons more readily upon light absorption. The ground-state acidity of the photoacid 2-naphthol can be significantly increased through coordination with Lewis acids such as boron trifluoride (BF). In this poster, we demonstrate that coordination with BF substantially suppresses the increase in acidity associated with photoexcitation. We achieved this through careful energy decomposition analysis (EDA) on the 2-naphtol-H2O and 2-naphtholate-H2O hydrogen-bonding complexes with and without an adducted BF3. We demonstrate that our computational results are in good qualitative agreement with the conclusions reached through absorption and fluorescence spectroscopy in Jahan Dawlatys lab. Overall, our work provides new insights into how Lewis acid coordination influences the photochemical behavior of aromatic photoacids.

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Poster 26:

*Experimental and Computational Study of the Growth Mechanism of Silver Nanoparticles by Borohydride Reduction*

**Tatyana D'Alessandro, Rocco Ammirata, and David Pullman**
San Diego State University

The synthesis of silver nanoparticles in aqueous solutions via the reduction of silver ions by sodium borohydride has been widely used for many decades. Nonetheless, the mechanism of the reaction and in particular the initial stages of silver nanoparticle formation remain largely unknown, both experimentally and computationally. This lack of mechanistic information is surprising, given its potential value in optimizing the chemical and physical properties of the resulting nanoparticles. The goal of the current project is to determine the reaction mechanism by identifying the chemical intermediates. The main experimental challenge is the reactions speed: it is complete after only one second, making detection of intermediates difficult. To address this, our group designed and constructed a rapid-mixing reactor integrated with a fast UV-visible absorption spectrophotometer capable of recording spectra on a millisecond timescale. A key result is the occurrence of an absorption peak at 240 nm which grows from the moment of reaction initiation, then decays as a second peak that is characteristic of semi-spherical silver nanoparticles begins to grow at 400 nm. An isosbestic point at 340 nm is observed, which indicates the 240 nm peak belongs to an intermediate species. The question now is: what is the chemical identity of this intermediate? Other experimental methods have not been able to answer this question. To help identify this species, we are performing TD-DFT computations on various potential species in solution and comparing the simulated spectra with our experimentally obtained spectra. The quantum chemistry software packages ORCA and Molpro were used. Before TD-DFT calculations could be performed, a suitable functional and basis set needed to be determined. Optimized geometries, thermochemical properties, and simulated UV-visible absorption spectra of small silver-containing molecules and clusters were calculated using a variety of functionals and compared with reference data-experimental data when available, and CCSD(T)-F12b/aug-cc-pVTZ-PP-F12 results when experimental data were not available. We find that results obtained at the revDSD-PBEP86-D4/minimally-augmented-def2-qzvpp level of theory show the greatest similarity to the reference data. Once the functional and basis set were chosen, the TD-DFT simulations of potential species in the reactant mixture were conducted. The species include silver atoms and ions, silver clusters, and combinations of these species with hydrides, borohydrides, hydroxides, oxides, and borates. Of these possible species, only silver hydride clusters and clusters containing silver and borohydride show spectra that roughly match the experimental spectra. Specifically, the spectra show a peak in the low-to-mid-200nm region, but not near 400nm. Importantly,

silver clusters–even a silver dimer–have both characteristic peaks, indicating that the intermediates are not simply silver clusters. Silver clusters with hydroxides or oxides similarly absorbed at higher wavelengths than those at which the intermediate species absorbs. Our TD-DFT work leads us to the present conclusion that the intermediates are either silver hydride or silver borohydride clusters, which ultimately decay into silver clusters and eventually form silver nanoparticles.

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Poster 27:

*Density Functional Theory Studies of Hyperfine Coupling in Sc(II) Complexes*

**Eric Ma, Thomas N. Panella, Ellie K. Byun, Filipp Furche**

UC Irvine

The recent emergence of Sc(II) metallocenes provides a productive platform to probe the influence of ligand environments on hyperfine coupling of rare-earth metals. To this end, new complexes of Sc(II) have been synthesized using 1,3,4,5-tetramethylimidazole-2-ylidene ($IMe_4$) and 4-dimethylaminopyridine (DMAP). Herein, the $^{45}$Sc hyperfine coupling constants of $(C_5Me_5)_2Sc(IMe_4)$, $(C_5Me_5)_2Sc(IMe_4)(CO)$, $(C_5H_2(^tBu)_3)_2Sc(IMe_4)$ and $(C_5H_2(^tBu)_3)_2Sc(DMAP)$ are studied using density functional theory (DFT) calculations. Molecular orbital analysis indicated increased Sc-centered s character that contributed to larger hyperfine coupling from ligand coordination. Comparisons with hypothetical complexes with isoelectronic ligands provide further insight on the possible factors contributing to this effect.

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Poster 28:

*Benchmarking DFT-Based Electronic Couplings in Saturated Donor-Bridge-Acceptor Systems: Distance and Conformational Effects*

**Hridita Purba Saha, Shaama Mallikarjun Sharada**

University of Southern California

Marcus theory is widely used to describe electron transfer kinetics. In the nonadiabatic regime, the rate depends quadratically on the donor-acceptor electronic coupling, so reliable rate predictions require accurate couplings. Previous benchmarks of DFT-based coupling methods have focused mainly on donor-acceptor dimers. Here, we extend this assessment to covalently linked donor-bridge-acceptor (D-B-A) systems consisting of a biphenylyl donor and a 2-naphthyl acceptor joined by saturated cyclohexane, decalin, and steroid bridges. These systems let us probe how donor-acceptor separation and attachment geometry, axial versus equatorial, affect the coupling. Reference couplings were derived from electron transfer rate constants measured by pulse radiolysis. We compare five approaches: direct coupling between constrained DFT (CDFT) states, generalized Mulliken-Hush (GMH), CDFT configuration interaction (CDFT-CI), fragment-orbital DFT (FODFT), and the fragment molecular orbital (FMO) method. To span Jacob's ladder of density functional approximations, we selected a GGA-based and a meta-GGA-based functional from each rung: PBE and B97M-V (semilocal), PBE0 and M06-2X (global hybrids), B97X-D and B97M-V (range-separated hybrids), and B97X-2(LP) and B97M(2) (range-separated double hybrids). All calculations were performed in implicit tetrahydrofuran (THF, PCM) with the 6-311+G** basis set, using B97X-D/6-311+G** optimized geometries. For equatorial-equatorial (ee) isomers, direct CDFT coupling (M06-2X) and GMH (PBE0) agree best with experiment, with mean absolute percentage errors of 18% and 12%. Both reproduce the exponential decay of coupling with the number of bridging bonds ( = 1.31 and 1.23 bond versus 1.17 bond experimentally). CDFT-CI (B97M-V) underestimates coupling magnitudes by about 94% but still captures the distance trend qualitatively ( = 0.89 bond). The fragment-based FMO and FODFT methods show decay roughly twice as steeply as experiment ( = 2.56 and 2.21 bond), consistent with an incomplete description of bridge-mediated superexchange. For conformers with axial attachment (ae, ea, aa), errors of direct CDFT, GMH, FODFT and FMO are substantially larger and vary strongly with geometry. In contrast, the CDFT-CI (B97M-V) error remains nearly uniform across all configurations,

with an average underestimation of 93%, pointing to a systematic rather than geometry-dependent origin. These results show that geometry-sensitive through-bond pathways remain a key challenge for predicting couplings in flexible D-B-A systems.

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Poster 29:

*The Best $\mathcal{O}(N^5)$ Scaling Excited State Method? The Linear Response of the Approximate Second Order Coupled-Cluster Method With Size Consistent Brillouin-Wigner Repartitioning*

**Jason Tae Yi, C. William McCurdy, Martin Head-Gordon**

UC Berkeley

The accurate calculation of electronic excitation energies is a challenging problem, but central to modeling photochemistry. One of the most accurate method used is the equation-of-motion (EOM-) or linear response of (LR-) coupled-cluster method with single and double substitutions (CCSD). Although EOM-CCSD is achieves high accuracy for vertical electronic excitations, it has a formal computational complexity of $\mathcal{O}(N^6)$ which can be prohibitively expensive for even moderately sized systems (i.e. $\geq 10$ heavy atoms). The approximate second order coupled-cluster method (CC2) has been previously introduced to reduce the cost of CCSD to $\mathcal{O}(N^5)$ while maintaining similar accuracy. CC2 and its EOM- and LR- variants are successful and widely used, but they fail to be regular theories for systems with strong static correlation at their equilibrium geometry or with a vanishing HOMO-LUMO gap. Recently Fink and Head-Gordon introduced the second order Brillouin-Wigner perturbation theory with size consistent repartitioning (BW-s2) which is a regular and size consistent $\mathcal{O}(N^5)$ correction to the ground-state energy with similar accuracy to second order Møller-Plesset perturbation theory (MP2). BW-s2 achieves size consistency by modifying the zeroth order Hamiltonian (i.e. the Fock matrix) in BWPT to include a one-body regularizer which eliminates disconnected terms through second order. Repartitioning the zeroth order Hamiltonian of CC2 to include the BW-s2 regularizer returns a regular and size consistent formulation of CC2, hereafter denoted BWs-CC2. The BWs-CC2 ground-state has been explored previously and was found to have similar energetics to CC2 but with the benefit of regularity. Additionally, BWs-CC2 accurately calculates the ground-state energy of $H_2$ in STO-3G (2-in-2 model) at dissociation. In this work, we present the linear response of the BWs-CC2 wave function, hereafter denoted LR-BWs-CC2. LR-BWs-CC2 is a regular, size consistent, $\mathcal{O}(N^5)$ excited state method with fascinating properties. Firstly, the excitation spectrum of LR-BWs-CC2 interpolates between CC2 (no regularization) and configuration interaction singles (CIS) (infinitely strong regularization). Additionally, BWs-CC2 achieves exactness in the 2-in-2 model for all electronic states at dissociation. Benchmarking of LR-BWs-CC2 vertical excitation energies against 423 data points reveals it performs better than CC2 for most excitation characters, with marked improvement on Rydberg, triplet, and charge transfer excitations. Our findings suggest that LR-BWs-CC2 is the best known $\mathcal{O}(N^5)$ scaling excited state method for vertical excitation energies.

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Poster 30:

*Internal conversion in polyatomic molecules: Theory, Implementation, Benchmarks and Diagnostics*

**Harsh Aryan Jalan and Anna I. Krylov**

University of Southern California

Internal conversion (IC) is a non-radiative relaxation process of electronically excited states. It competes with fluorescence and controls excited-state lifetimes and quantum yields. Calculations of IC rates involves evaluation of Franck–Condon factors (FCFs) and vibrational density of states. Hence, predicting IC rates in polyatomic molecules is difficult. I will present a time-domain theory of computing IC rates based on vibrational FCFs and non-adiabatic couplings (NACs) from electronic-structure calculations. Starting from Fermi's Golden Rule within the Born–Oppenheimer, harmonic, and Condon approximations, we recast the Franck–Condon weighted density of states (FCWD) as the Fourier trans-

form of a vibrational correlation function and show that it is identical to the energy-domain sum over final vibrational states. We compared computed rates with measured IC rates for seventeen molecules, including azulene and its derivatives, the polyacenes, and the *N,N*-dimethylaminonaphthalenes. For six azulene-type chromophores, our rates agree with experiment to within one order of magnitude, about two orders closer than the effective-mode model of Shi, Xie, and Troisi. Our method underestimates the polyacene rates by about two to seven orders, even at the experimental energy gap. Displacing anthracene along its normal modes activates NAC components that vanish at equilibrium, whereas the NACs of guaiazulene remain nearly constant. This points to Herzberg–Teller coupling, which we will add to the theory. Our method also underestimates the *N,N*-dimethylaminonaphthalene rates by 11 to 13 orders, because these molecules decay through twisted charge-transfer structures that lie beyond a **single harmonic minimum. In this poster, I will present the theory, its benchmark against experiment, and how its failures guide these planned extensions toward predictive IC** rates.

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Poster 31:

*Thermodynamically Consistent Coarse-Graining of Molecular Systems: Beyond Rigid-Monomer Models*

**Joao V. M. Pimentel; Vladimir A. Mandelshtam**

UC Irvine

We present a framework for coarse-graining molecular systems that selectively groups atoms that belong to relatively rigid subunits (e.g., entire molecular monomers or segments of larger molecules) and directly constructs a free energy function depending on the centers and orientations of these subunits, i.e., the coarse-grained (CG) coordinates. Unlike conventional rigid-body approaches, the internal configurations of the subunits are not fixed. Starting with an all-atom potential, the configuration space is partitioned into the slow (CG) and fast subspaces. The fast degrees of freedom are averaged out using a local harmonic approximation, producing a temperature-dependent CG free energy that has the option of including nuclear quantum effects in the fast subspace. Despite its conceptual simplicity, the approach yields remarkably accurate equilibrium properties for water and ammonia clusters. The CG simulations achieve statistical convergence with fewer sampling steps, and the cost of a single free energy evaluation remains comparable to that of the original all-atom potential.

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Poster 32:

*The Performance of Machine-Learned Universal Model for Atoms Potentials on Acid-Base Multicomponent Crystals*

**Aerial Bridgers-Anguiano, Greg Beran**

UC Riverside

Acid-base multicomponent crystals (ABCs) provide a path for increasing the solubility of active pharmaceutical ingredients (APIs). ABCs can appear as a salt, cocrystal, or intermediate form based on the location of the proton between components. Accurately determining the position of the proton between the acid-base components remains challenging both experimentally and computationally. Generalized Gradient Approximation Density Functional Theory (GGA DFT), typically utilized in crystal structure prediction studies (CSP), is known to suffer from density-driven delocalization error, resulting in spurious stabilization of the salt form. Acid-base pair energy corrections, in which the periodic crystal is treated with low-level and less expensive GGA functionals while the key intermolecular acid-base interactions are treated with more accurate density functionals, were shown to successfully mitigate the erroneous salt stabilization. However, correct ABC category assignment relies on optimizing several structures along the proton transfer path, which is expensive even with low-level density functionals. The development of machine-learned interatomic potentials (MLIP), such as the Universal Model of Atoms (UMA), can reduce the of crystal optimizations from days to minutes, but this MLIP has not been verified for ABCs. Here, we show that optimizing the structures along the proton path with UMAs

Open Molecular Crystal (OMC) performs analogous to a GGA, but correcting OMC energies with Open Molecules (OMol, an MLIP trained on a higher density functional) produce inconsistent results from ABC to ABC. However, applying the energy corrections with DFT on the OMC optimized structures remains accurate and cost-effective.

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Poster 33:

*Understanding the Impact of Pore Electronic Structure on Nanoconfined Ion Transport*

**Edward Chen, Kara Fong**

California Institute of Technology

Ion transport through nanopores is central to energy storage and selective ion separation. Although the electronic response of confining surfaces can alter ion interactions, its influence on collective ion transport remains incompletely understood. Here, we use molecular dynamics simulations of aqueous sodium chloride confined to a single molecular layer to isolate the role of surface polarization. Our model systematically varies only the electronic response of the confining walls, from ideally conducting to non-polarizable, while keeping pore geometry, electrolyte composition, and short range interactions fixed. As the wall response weakens, ions diffuse more slowly and cation-anion motion becomes more strongly correlated. Decomposing the conductivity into contributions from individual and correlated ion motion shows that correlations between like ions largely offset the decrease in self-diffusion, while stronger cation-anion correlations suppress charge transport. Structural analyses reveal increased contact ion pairing and a greater fraction of electrically neutral clusters under weakly polarizable confinement, consistent with the reduced conductivity. These results connect surface electronic response, ion association, and collective transport, identifying surface polarization as a means of tuning electrolyte behavior under extreme nanoconfinement.

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Poster 34:

*Exploring the Evolutionary Determinants of CRISPR-Cas Gene Editors through Interpretable AI and Free-Energy Simulations*

**Larry Rodriguez, Chinmai Pindi, Mohd Ahsan, Giulia Palermo***

University of California, Los Angeles

Despite remarkable advances in CRISPR-Cas genome editing, the molecular mechanisms by which directed evolution enhance the efficiency and function of gene editors remain poorly understood. Particularly, it remains unclear how evolutionary changes reshape protein interactions and conformational dynamics in prime editors (PEs) and adenine base editors (ABEs). Here, we combine molecular dynamics (MD) simulations with interpretable AI and enhanced sampling methods to investigate the molecular mechanisms and evolutionary determinants of recent PE systems (PE1, PE6d) and ABE8e. MD simulations were integrated with two complementary deep learning approaches: Graph Attention Networks (GATs) to uncover molecular interactions governing prime editor function, and Deep Linear Discriminant Analysis (Deep-LDA) to identify collective variables for enhanced sampling and free-energy simulations of ABEs. For prime editors, MD simulations combined with interpretable GATs reveal distinct RT-Cas9 interaction networks across conformational states of PE1 and PE6d, providing insights into the evolutionary remodeling of the RT-Cas9 interface. For ABE8e, we employ Deep-LDA to learn collective variables that distinguish relevant conformational states and enable enhanced sampling of their free-energy landscapes. This approach provides a framework for investigating how evolutionary changes reshape conformational preferences and molecular interactions underlying ABE function. Together, these studies demonstrate how interpretable deep learning and AI-driven free-energy simulations can uncover the molecular mechanisms through which directed evolution reshapes CRISPR-Cas gene editors, providing a foundation for the rational development of more efficient genome-editing technologies.

Poster 35:

*Non-adiabatic couplings within equation-of-motion spin-flip coupled-cluster framework: Theory, implementation, and examples.*

**Tingting Zhao, Xintian Feng, Shirin Faraji, Spiridula Matsika, Jürgen Gauss, and Anna I. Krylov**

University of Southern California

We present the theory and implementation of analytical nonadiabatic coupling (NAC) vectors for the equation-of-motion spin-flip coupled-cluster singles and doubles (EOM-SF-CCSD) method. We demonstrate the importance of the orbital-derivative contribution in the EOM-SF-CCSD ansatz and the role of proper normalization arising from the non-Hermitian nature of the theory. We compare our formulation with the previously derived Lagrangian-based expression and establish the equivalence of the two approaches. Furthermore, we introduce an efficient direct implementation with minimal modifications to the standard gradient formalism, in contrast to earlier sum-over-states approaches. As an application, we calculate NAC vectors along the C=C torsional coordinate of ethylene and compare the results with those obtained from multireference methods, demonstrating the performance of the EOM-SF-CCSD approach for describing nonadiabatic interactions.

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Poster 36:

*Making Gold (electron) Poor: A Benchmark of Coinage Metal Z-type Ligand Interactions*

**Samantha Chiang1, Linus Bjarne Dittmer2, Jason Tae Yi1,3, Martin Head-Gordon1,3, 1 Kenneth S. Pitzer Center for Theoretical Chemistry, Department of Chemistry, University of California, Berkeley, California 94720, USA 2 Interdisciplinary Center for Scientific Computing, Ruprecht-Karls University, Im Neuenheimer Feld 205, 69120 Heidelberg, Germany 3 Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA**

UC Berkeley

We present a high quality thermochemistry benchmark of complexes featuring dative bonds of coinage metals (CM) and Z-type ligands, organized into principal reaction categories. From an experimental point of view, CM/Z-type ligand (CMZ) interactions are of strong synthetic interest as they allow for tuning of electron density around molecular catalyst centers. However, from a theoretical point of view, CMZ complexes are highly underrepresented in benchmarks and are not included in training or validation datasets. We investigate the performance of common Density Functional Approximations (DFA) to describe these interactions, using selected reaction types chosen for their direct synthetic relevance or their suitability as reliable proxies. These include isodesmic reactions to approximate CMZ bond strengths, ligand exchange processes involving N-heterocyclic carbenes (NHC) which are widely used in transition metal catalysis as well as activation barriers for small-molecule transformations. We focus on the composition of the benchmark, establishing a much-needed predictive framework that aligns theoretical rigor with the practical demands of modern transition metal catalysis.

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Poster 37:

*Developing a Machine-Learned Force Field for Nonbonded Peptide-Bond Interactions: Beyond Training-Set Accuracy*

**Jiwon Huh, Ruihan Zhou, Francesco Paesani**

UCSD

Accurately describing long-range interactions remains a major challenge for state-of-the-art machine-learned force fields (MLFFs). The MB-nrg framework, developed by the Paesani group, addresses this challenge by explicitly incorporating long-range interactions through polarizable electrostatics and

damped dispersion, while capturing short-range quantum-mechanical effects through machine-learned corrections. This approach has demonstrated remarkable accuracy, extending the predictive capabilities of coupled-cluster theory from small molecular clusters to condensed-phase systems, as exemplified by the successful reproduction of the ice phase diagram using MB-pol. However, our investigation reveals that extending this framework to biomolecular systems is less straightforward than anticipated, primarily due to challenges in parametrizing the underlying classical interactions. Here, we develop a two-body MB-nrg potential for N-methylacetamide (NMA), a model compound for peptide bonds, and show that reproducing high-level electronic-structure cluster training data alone is insufficient to ensure physically reasonable condensed-phase behavior, highlighting the importance of charge parametrization and dispersion damping. Comparisons with other state-of-the-art MLFFs reveal broadly consistent radial distribution functions for liquid NMA, with variations reflecting differences in the underlying electronic-structure methods used for training, while the classical OPLS-AA force field exhibits substantially larger deviations. Potential energy surface scans further reveal significant errors and cutoff artifacts in MLFFs lacking explicit long-range interactions, highlighting limitations in their transferability beyond the local environments represented in their training data. These findings underscore the importance of physically motivated long-range interactions for developing accurate and transferable MLFFs for biomolecular systems.

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Poster 38:

*Molecular Simulations and Interpretable AI Reveal the Mechanistic Basis of TnsC Filament Assembly in CRISPR-Associated Transposons*

**Chinmai Pindi, Mohd Ahsan, Souvik Sinha, Elizabeth H. Kellogg, and Giulia Palermo**
UCLA

CRISPR-associated transposons (CASTs) enable programmable DNA integration, with the AAA+ ATPase TnsC playing a central role in coordinating transposition through the assembly of helical filaments on DNA. However, the molecular mechanisms governing TnsC filament nucleation, protein-DNA communication, and directional elongation remain poorly understood. Here, we combine large-scale atomistic molecular dynamics simulations, enhanced-sampling free energy calculations, Granger causality analysis, and interpretable graph attention networks (GATs) to elucidate the molecular basis underlying TnsC filament assembly in a type V-K CAST system. Our studies reveal that TnsC nucleation is initiated through interactions between the initiator-specific motif (ISM) and the DNA minor groove, inducing localized DNA deformation that propagates along extended filaments. Moving beyond conventional correlation-based analyses, Granger causality reveals directional predictive coupling between TnsC conformational dynamics and DNA remodeling. Specifically, motions of the ISM, Linker-2, and C-terminal regions precede and improve predictions of subsequent DNA structural changes, providing evidence for coordinated protein-DNA dynamics during filament formation. Free energy calculations and interpretable GAT models further identify the molecular interactions underlying the assembly, revealing a dominant recognition interface between the N-terminal region of the DNA-bound monomer and Linker 2 of the incoming monomer during the early stages of elongation. This initial recognition is followed by a reorganization of inter-subunit interactions that stabilizes the growing filament and regenerates the interface for subsequent monomer recruitment. Together, these findings uncover a dynamic mechanism in which protein-driven DNA deformation and directional inter-subunit communication govern processive filament growth. More broadly, our interpretable AI framework provides a transferable strategy for dissecting biomolecular mechanisms from molecular simulations.

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Poster 39:

*From Motion to Mechanisms: Edge-Aware Graph Attention Networks for Interpretable Molecular Dynamics*

**Mohd Ahsan, Chinmai Pindi, and Giulia Palermo**
UCLA

Molecular dynamics simulations generate extraordinarily rich descriptions of biomolecular motion, yet the interactions that actually organize these motions into folding, allostery, and assembly mechanisms are often buried within millions of correlated fluctuations. We developed an interpretable graph-attention framework that learns directly from MD trajectories and converts dynamical prediction into mechanistic insight. Biomolecules are represented as dynamic interaction graphs, and graph attention networks (GATs) are trained to predict how molecular configurations evolve in time. Rather than treating the learned attention as a black-box intermediate, we use it to identify interactions and residues that dominate dynamical information flow. Applied to CRISPR-associated TnsC filaments, this approach exposed early inter-subunit recognition events that precede productive filament elongation and revealed how the interaction network reorganizes as assembly progresses. We next asked whether explicitly encoding molecular physics into the graph edges could sharpen both prediction and interpretation. We therefore developed Edge-Conditioned, Edge-Injected, and Edge-Gated architectures that incorporate pairwise physical interaction features directly into attention and message passing. Across systems spanning protein folding, allosteric regulation, and large biomolecular assemblies, edge-aware models recover distinct layers of mechanism that are obscured by structure-only representations. In Chignolin, attention networks identify interactions associated with the folding; in HIV-1 protease, they resolve mutation-dependent rewiring between distal regions, the flaps, and the active site; and in TnsC assemblies, they capture interaction patterns associated with oligomerization and filament growth. These results suggest that graph attention can serve not only as a predictor of molecular motion, but as a microscope for interrogating it. By transforming MD trajectories into residue-level, physically grounded interaction networks, edge-aware GATs provide a general framework for discovering the molecular pathways that connect structure, dynamics, and function.

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Poster 40:

*Transition Metal and Photobase Complex: Excited State Proton Transfer (ESPT)*

**Hayden Harkins, Dr. Andrew Petit, Dr. Jahan Dawlaty, Sophia Duong, Rosa Figueroa**
Cal State University Fullerton

Photobases are underutilized, compared to photoacids, due to their short-lived excited state lifetimes and the need for multiple hydrogen bond partners to stabilize the product of excited-state proton transfer (ESPT). If these limitations can be overcome, it opens the door for many applications including catalysis and photo-energy harvesting. To overcome these limitations, we explore attaching a pendant photobase to a transition metal complex containing Zn2, Ni2+, or Pt2+. The reactant, an amine with a phenyl group, binds to the transition metal center, which pre-organizes it into a hydrogen-bonding configuration with the photobase. We show that we can selectively excite the photobase and that this photoexcitation facilitates ESPT. The metal plays an important role in this process by stabilizing the anion generated through ESPT. We further propose a fluorescence-based approach to experimentally determining whether ESPT occurs.

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Poster 41:

*Solvent effects on the spin dynamics of the semiquinone radical anion in solution.*

**Rayirth Bhatt, Eleftherios Lambros**

California State University, Fullerton

Quantum computers store information using foundational units called qubits. The conventional qubits that are in use today are highly susceptible to thermal fluctuations and typically require extreme cryogenic temperatures to maintain stability. In contrast, stable organic semiquinone radical qubits function as viable molecular alternatives while remaining stable at ambient temperatures. This research investigates the influence of solvent environments, such as water, on these semiquinone molecules. In this study we examine the spin dynamics of semiquinone molecule using real-time TDDFT simulations, directly examining the electronic spin dynamics. Initially, the spin dynamics are evaluated in a vacuum, followed by comparative analyses in a solvent environment. Alterations in spin precession frequency serve as a direct indicator of molecular stability for qubit applications in quantum computing.

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Poster 42:

*Visualization Tools for Relativistic Quantum Chemical Software*

**Matthew Hitt, Eleftherios Lambros**

California State University, Fullerton

The Chronus Quantum software package (ChronusQ), developed by the University of Washington, is a tool for simulating modern electronic structure under time dependence. With an interest in analyzing spin density for various organic radicals, we develop visual and mathematical tools for the analysis of electronic structure calculations, by linking ChronusQ to popular visualization software such as UCSF ChimeraX through an add-in module. This will help support the analysis of chemical simulations and allow for greater study of relativistic and spin dependent systems such as organic radicals in order to achieve stable, room-temperature qubits in the future.

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Poster 43:

*Investigating Nitrogen Monoxide as a CISS Reporter for Propylene Oxide and Butanol Systems*

**Joshua Valdez, Bennett Clark, Garrett Burroughs, Joshua Kerrigan, Andrew S. Petit, Nathan Kidwell**

California State University, Fullerton

Chirality-induced spin selectivity (CISS) is a phenomenon in which molecular chirality gives rise to spin-selective effects, such as preferential transmission of one electron-spin orientation over the other. Previous theoretical work in the Krylov group investigated this effect in a chiral photoswitching molecule and identified differences in the matrix elements of the spin-orbit coupling Hamiltonian (HSOC) as an important contributor to enantiomer-dependent spin dynamics. Importantly, these calculations neglected any contributions to the CISS effects associate with molecular vibrations.

This poster investigates nitrogen monoxide (NO) as a radical probe of spin-vibronic effects associated with CISS in intermolecular complexes of NO with propylene oxide and 2-butanol. Experiments performed in the Kidwell group monitored the final quantum state of NO obtained from the vibrational dissociation of the complex. The experimentally observed rotational distribution of the NO exhibited a clear dependence on which enantiomer the NO was interacting with. Our objective is to examine how intra- and intermolecular vibrational motions influence spin polarization in these systems. In particular, calculations using the NO-propylene oxide complex reveal that the spin-orbit coupling matrix elements depend on the relative rotational orientation of NO. We further demonstrate a non-zero difference in the spin-polarization of NO depending on which enantiomer it is interacting with. This difference in the spin polarization varies considerably along intermolecular wagging modes. These findings provide insight into the interplay between molecular geometry, spin-orbit coupling, and spin-vibronic effects in

CISS systems.

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Poster 44:

*Tracking the Evolution of Electronic Character of Ground and Excited States with Mixed-Reference Spin-Flip TDDFT*

**Arnab Chakraborty, Zheng Pei, Yihan Shao, and Anna I. Krylov**

University of Southern California

Molecular torsion and increasing conjugation length can change the electronic character of ground and excited states, often introducing substantial multiconfigurational character. Describing these changes requires both an efficient electronic-structure method and analysis tools that go beyond excitation energies. Mixed-reference spin-flip time-dependent density functional theory (MRSF-TDDFT) extends the applicability of standard TDDFT to strongly correlated states while substantially reducing the spin contamination associated with original spin-flip TDDFT. We present an efficient implementation of MRSF-TDDFT in Q-Chem, providing excitation energies, oscillator strengths, spin-orbit couplings, and transition density matrices. Integration with libwfa enables density-based characterization using natural orbitals, natural transition orbitals, natural difference orbitals, and excitonic descriptors. We first examine how electronic character changes with molecular geometry, following the evolution of diradical character along torsion in tetramethyleneethane and examining the ground and first excited singlet states near a conical intersection in the retinal model PSB3. Comparisons with high-level wave function calculations assess the description of these states, while spin-orbit couplings in selected diradicals demonstrate the effectiveness of the approach. We then turn to two important families of conjugated systems, polyenes and polyacenes, to follow changes in single-excitation character and exciton descriptors in their low-lying valence states with increasing conjugation length. Together, these studies show how MRSF-TDDFT equipped with density-based analysis helps reliably interpret trends in state energies and spectroscopic properties and follow changes in electronic character as states mix and change order.

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Poster 45:

*Analyzing Condensed-Phase Bond Breaking and Decoherence via Polarizability*

**Riley Wexler and Benjamin J Schwartz**

UCLA

When a coherent quantum system interacts with a fluctuating environment, such as a liquid, solvent-solute interactions can induce decoherence, collapsing the system into a non-coherent eigenstate. Previously, we have investigated this phenomenon using the dissociation of a photoexcited sodium dimer cation in liquid argon as a model system, revealing that a minimum bond distance of 8  is required for asymmetric solvent-solute collisions to initiate decoherence. However, the physical origin of this specific spatial threshold has remained unclear, largely due to broader ambiguities in precisely defining the bond breakage point. Recently, Hait and Head-Gordon demonstrated that bond parallel polarizability can be used to unambiguously identify these bond breakage points in ground-state gas-phase systems. In this work, we extend this concept to the condensed phase. Crucially, while polarizability is unbounded during dissociation in the gas phase, it becomes strictly bounded in the condensed phase due to interactions with the surrounding solvent. Thus, by analyzing how the solvent bounds this polarizability, we propose a physical origin for the 8  threshold required for asymmetric collisions to initiate decoherence.

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Poster 46:

*Intrinsic Helicity of a Modified Sugar-Phosphate Backbone: Computational Analysis of Imidazole-Substituted DNA Analogs Derived from a DNA/RNA Hybrid*

**Iftykhar Ifty and Marcos Alvarez**

Los Angeles Mission College

The double-helical structure of nucleic acids arises from base pairing, base stacking, backbone torsional preferences, and solvation. Separating the contribution of each factor to the overall helical geometry remains an open question in structural chemistry. In this work, we investigate the intrinsic helical character of the sugar-phosphate backbone by systematically removing and replacing the nucleobases in a crystallographically characterized nucleic acid structure and tracking quantitative helicity descriptors through each stage of modification and quantum-mechanical geometry optimization. The starting structure is derived from PDB entry 479D, a nine-nucleotide DNA/RNA hybrid duplex. Chain B, originally an RNA strand, is first converted to DNA by replacing each ribose 2'-OH with hydrogen. The natural bases on both chains are then removed and replaced with imidazole groups, producing a minimal backbone analog in which Watson-Crick base-pairing is eliminated, and the large-scale stacking interactions of natural nucleobases are replaced by the weaker stacking capacity of a single five-membered aromatic ring. This substitution series  original hybrid, all-DNA conversion, base-free backbone, and imidazole-substituted backbone  provides a stepwise decomposition of the forces that maintain helical geometry. Each structure is optimized at the r2SCAN-3c/CPCM(Water) level of density functional theory using ORCA 6.1, and the optimized geometry is validated by vibrational frequency analysis at the same level. Helical character is measured at every stage using a set of geometric descriptors calculated from the sugar-ring center points and phosphorus positions along the backbone. These descriptors include the backbone extension index, axial monotonicity, mean phosphate rotation angle, residues per turn, helical pitch, and phosphate radius from the molecular axis. By comparing these descriptors before and after optimization and across the substitution series, we assess how much helical character is retained by the backbone alone. Preliminary reference calculations on an optimized eight-residue imidazole-bearing chain give a mean phosphate rotation of approximately 89 degrees with 4.0 residues per turn and a pitch of 22.9 angstroms. In comparison, an optimized base-free chain gives approximately 79 degrees with 4.5 residues per turn and a pitch of 25.2 angstroms. For comparison, canonical B-form DNA has approximately 36 degrees per residue, 10 residues per turn, and a pitch of 34 angstroms. The modified backbones therefore adopt a much tighter helix, but these values indicate that significant helical structure is maintained in the sugar-phosphate framework even when natural nucleobases are absent or replaced. Ongoing calculations on the nine-nucleotide 479D-derived structures for both Chain A and Chain B will extend this analysis to a crystallographically grounded starting geometry and allow direct comparison between the DNA and modified-RNA backbones.

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Poster 47:

*CISS Effect Through the Lens of Spin Density Differences*

**Jia Hao Soh and Anna I. Krylov**

University of Southern California

Chirality-induced spin-selectivity (CISS) is the preferential transport of electrons of one spin over another due to the handedness of the molecular system. CISS has many applications, for example, in catalysis, photovoltaics, and quantum information science. Experimental studies have documented the CISS effect in various setups; however, these involve complex systems such as surfaces and large molecules, and as such, no clear and unified theoretical framework based on first-principles approaches has been established to identify the fundamental principles of the CISS effect.

Existing works show that chiral photoswitching molecules can describe CISS with first-principles approaches through purely electronic transitions. However, it remains unclear how large biomolecules such

as DNA can exhibit a large CISS effect without containing heavy elements. RAO (riboaminooxazoline), an RNA precursor, is one such biomolecule, which exhibits a large CISS effect through enantioselective crystallization on a magnetized magnetite surface. To explain this quantitatively, we analyze electronic states of the RAO–Cs system using high-level quantum chemistry methods. We compute electronic states using state-interaction approach including spin-orbit coupling and Zeeman effect. As a visual to illustrate these perturbations, we compute and plot spin densities to illustrate the difference in electron occupation between the spin-orbit states.

References: [1] C. Seibel, J. H. Soh, S. Zilberg, and A. I. Krylov, J. Phys. Chem. Lett. 2025, 16, 33, 8514-8522 [2] S. Furkan Ozturk, Z. Liu, J. D. Sutherland, and D. D. Sasselov, Sci. Adv., 2023, 9, eadg8274

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Poster 48:

*The Influence of Water as a Guest Molecule on the Spin Dynamics of DAT-DBA*

**Jacob Nguyen, Eleftherios Lambros**

California State University Fullerton

Metal Organic Frameworks (MOFs) are a class of stable organic radicals which have shown promising signs of being a candidate for spin qubits for quantum computers due to their higher coherence times and stability at room temperature. Several MOF qubits have successfully been synthesized, yet there are many open questions on physics underlying this stability. This work aims to investigate a specific MOF ligand known as DAT-DBA and dissect its behavior with and without a guest water molecule at 3 different key positions. Using real-time time-dependent density functional theory, we investigate how water binding at different positions on the DAT-DBA linker influences the quantum spin dynamics of this molecular qubit.

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Poster 49:

*Polarization is Required to Model Electrostatic Preorganization: The Case of Chorismate Mutase*

**Giacomo Berti, Pujan Ajmera, Anastassia N. Alexandrova**

UCLA

Electrostatic preorganization contributes to enzymatic catalysis through transition state stabilization and is often investigated using classical molecular dynamics (MD) simulations that employ fixed-charge force fields (FFs). Although polarizable FFs allow for more accurate quantification of local electrostatic effects, whether they qualitatively differ from fixed-charge FFs regarding more global properties, such as the substrate conformation stabilized by the enzyme's electrostatics, remains unclear. Here, we compare molecular dynamics simulations of chorismate mutase performed with the AMOEBA polarizable FF and the AMBER fixed-charge FF. We find that simulations using AMOEBA sample chorismate geometries resembling the transition state-like near attack conformation (NAC), while AMBER simulations sample predominantly non-NAC conformations. The local substrate-protein interactions are also completely altered by the choice of FF, with AMOEBA and AMBER each sampling distinct active site hydrogen bond networks. Finally, even at matched reactive substrate conformations, the heterogeneous three-dimensional electric field experienced by the substrate is qualitatively different between the FFs. By additionally comparing to a modified AMOEBA FF with the induced dipole term turned off, we also isolate the explicit polarization in AMOEBA as a key contributor to these differences. Our results highlight the importance of explicitly accounting for polarizability in classical simulations, with implications for MD-based screening methods and the use of MD frames to seed further analyses.

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Poster 50:

*Extracting Molecular Dynamics from Ultrafast Diffraction*

**Roya Moghaddasi Fereidani, Wanlu Li, and Haiwang Yong**

University of California, San Diego

Ultrafast electron and X-ray diffraction provide powerful experimental probes of molecular structural changes during photochemical reactions. However, reconstructing time-dependent molecular geometries and reaction pathways from diffraction signals remains a challenging inverse problem, particularly when multiple molecular configurations contribute to the measured signal. Here, we present non-AI and AI-based approaches using physics-constrained forward optimization and deep learning to extract molecular structures and dynamics from ultrafast diffraction measurements.

First, we employ a trajectory-based forward-optimization framework to investigate the photoinduced ring-opening reactions of isoxazole and oxazole. Nonadiabatic surface-hopping simulations provide ensembles of physically accessible molecular trajectories, from which electron diffraction signals are calculated. After accounting for the experimental instrument response, the statistical weights of individual trajectories are optimized to minimize the discrepancy between simulated and experimental diffraction signals. This non-AI approach preserves the temporal continuity of molecular dynamics while reconstructing time-dependent structural distributions and reaction branching populations. Our results reveal distinct ring-opening mechanisms in isoxazole and oxazole, demonstrating how subtle changes in heteroatom positioning influence ultrafast photochemical dynamics.

To overcome the need for extensive nonadiabatic surface-hopping simulations, we developed two deep-learning approaches to directly reconstruct 3D molecular structures from diffraction signals. The first is a deterministic model combining a convolutional neural network that encodes diffraction signals with an equivariant graph neural network that learns molecular geometry representations. The two encoders are trained through latent-space alignment, and a shared multilayer perceptron reconstructs atomic coordinates. The second approach is a conditional generative model based on a denoising Transformer and flow matching. A convolutional neural network encodes the diffraction signal, while atomic identities and generative-time embeddings condition the transformer to progressively transform Gaussian noise into molecular geometries. Unlike deterministic reconstruction, this generative approach can produce multiple candidate structures consistent with a given diffraction signal, providing a framework for exploring structural ambiguities.

Our ultimate goal is to develop a universal deep-learning framework capable of reconstructing three-dimensional molecular geometries directly from ultrafast diffraction signals and atomic numbers. By learning a generalizable mapping between diffraction patterns and molecular structures, we aim to extend this framework to a wide range of molecules and enable efficient reconstruction of molecular structures and dynamics from experimental measurements.

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Poster 51:

*Many-Body Modeling of Aqueous Azide: From Local Interactions to Hydration Structure*

**Zhenkun Chen, Jiwon Huh, Francesco Paesani**

UCSD

Hydration of molecular ions is governed not only by ion-water contact distances but also by directional interactions and collective solvent organization. The linear azide anion (N) provides a useful system for investigating how local many-body energetics influence the structure of the surrounding aqueous environment.

In this work, we develop and evaluate an azide-water interaction model within the MB-nrg framework, combining high-level electronic-structure reference calculations, short-range permutationally invariant Fourier series (PIFS) representations of two-body (2B) and three-body (3B) interactions, and many-body polarization. The model is systematically assessed through electronic-structure energy

benchmarks, direction-resolved potential energy surfaces, and molecular dynamics simulations of aqueous azide.

Our analysis reveals that improvements in the local directional energetics of azide-water interactions do not necessarily produce corresponding changes in the overall hydration structure. In contrast, incorporating explicit short-range three-body interactions leads to more pronounced changes in hydration-shell occupancy, water packing, and spatial organization, while the characteristic ion-water contact distances remain largely unchanged. Furthermore, changes in local solvent density do not always correspond to changes in the total hydration-shell population, highlighting the distinction between local concentration and collective solvent organization.

These findings demonstrate the importance of connecting accurate local interaction models with their emergent condensed-phase behavior. By examining the relationship between many-body energetics and hydration structure, this work provides physical insight into the organization of water around molecular ions and illustrates the limitations of inferring collective hydration behavior from isolated ion-water interactions alone.

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Poster 52:

*Revealing Structure-Function Relationships Involving Substituent Positions for Isoquinoline Photobases*

**Viktoria Silva,Joshua Valdez,Claudia Ramos,Megan Warner, Dara Varasteh, Samantha de Pozo,Ryan Hunt, Andrew S. Petit**

California State University, Fullerton

Photobases are molecules that become significantly stronger bases upon photoexcitation. Structure-function relationships for 5-substituted quinolines have been thoroughly studied in earlier experimental work, which has shown that the thermodynamic driving force for excited-state protonation gets stronger as the substituent becomes more electron-donating. Potential photobasicity descriptors involving intramolecular charge-transfer, excited-state antiaromaticity relief, and energy decomposition analysis (EDA) in the 5-substituted quinoline series were investigated in previous computational work. However, the literature lacks a thorough examination of how shifting substituent location can impact photobasicity strength. In this study, we bridge the gap by experimentally showing that the position of the bromine atom considerably modulates the ground-state and excited-state basicity of bromoisoquinolines. Descriptors based on intramolecular charge-transfer, excited-state antiaromaticity relief, and EDA are applied in complementary computational studies. We show that EDA provides a robust descriptor of photobasicity across both the 5-substituted quinolines and the bromoisoquinolines.

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Poster 53:

*Revealing imatinib-kinase specificity via analyzing changes in protein dynamics and computing molecular binding affinity*

**William Troxel, Emily Vig, Chia-en A. Chang**

University of California, Riverside

Drug promiscuity is a double-edged sword where a small molecule acts on multiple biological targets to induce toxicological or therapeutic benefits. It is possible to exploit promiscuity to expand treatment options without the prohibitive costs of designing a new drug. Imatinib is a representative case, exhibiting varied affinities and inhibitions to different kinases. It binds most favorably to Abl and Kit kinases, intermediately to Chk1 and Lck kinases, and least favorably to p38 and Src kinases. The strongly conserved features of the ATP-binding site render imatinibs molecular binding determinants unclear despite over 25 years of interrogation. To address this question, molecular thermodynamics, force distribution analysis, residue sidechain dihedral correlations, and principal component analysis were computed using trajectories from all-atom molecular dynamics simulations in explicit solvent. The results of these simulations agree with experimental affinity and binding data, enabling highly

predictive factors for imatinibs binding specificity from free- and bound-state simulations through a global protein network of protein-ligand interactions, changes in sidechain dihedral correlations, and shifts in the secondary motifs modulating binding site access corresponding with well-characterized kinase breathing motions. The sidechain dihedral correlation network also identifies distal mutants known to reduce patients imatinib sensitivity. Higher imatinib-kinase affinity trends with a loss in sidechain dihedral correlations and diminished secondary motif migration following binding, corresponding with more restricted configurations, to reduce solvent approach and ATP competition. Lower-affinity proteins show enhanced sidechain dihedral correlation and exaggerated secondary motif motions. This is consistent with a tendency to expose the protein pocket, facilitate solvent entrance, and increase ATP competition. Using imatinib as a model system, this study shows residue correlation, force interaction, and essential principal components can effectively forecast imatinib-kinase binding specificity and introduces an effective approach to repurpose and design high-affinity binders for off-target applications more generally.

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Poster 54:

*Hyperfine Coupling as a Fingerprint of Reduction in Scandium Metallocenes*

**Shan Yi, Ahmadreza Rajabi, and Filipp Furche**

University of California, Irvine

One-electron reduction of scandium(III) metallocenes can result in either metal-centered or ligand-centered electronic structures, depending on the coordinated ligand. Distinguishing these reduction pathways is essential for understanding the electronic properties and reactivity of reduced scandium complexes. In this work, density functional theory (DFT) calculations were employed to investigate the electronic structures and spectroscopic properties of five reduced scandium metallocenes. Geometry optimizations, molecular orbital analysis, natural spin population analysis, and time-dependent DFT calculations were combined with relativistic calculations of electron paramagnetic resonance (EPR) parameters to characterize their electronic structures.

Our results reveal two distinct reduction patterns. Complexes **1, 2, and 5** exhibit predominantly metal-centered reduction, characterized by substantial Sc 3d spin density and a formal Sc(II) (3d) configuration. In contrast, complexes **3 and 4** undergo predominantly ligand-centered reduction, retaining a formal Sc(III) (3d) center. Calculated scandium hyperfine coupling constants successfully distinguish these electronic structures, with large couplings for metal-centered radicals and substantially smaller values for ligand-centered radicals, consistent with experimental EPR measurements. Further conformational analysis of complex 4 identifies a lower-energy ligand-centered structure, favored by 6.90 kcal mol over an alternative metal-centered conformer. Simulated UV-Vis absorption spectra provide complementary insight into the electronic transitions of these complexes.

Overall, these findings demonstrate that scandium hyperfine coupling serves as a sensitive spectroscopic fingerprint for identifying reduction sites in scandium metallocenes and highlight the important role of ligand electronic structure in controlling reduction behavior.

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Poster 55:

*Quantum Chemical Study of Graphene-Based Hydrogen Storage Using Benzene as a Model for Graphene*

**Jonathan Lu, Dr. Fu-Ming Tao**

CSUF

Graphene's extended -electron system makes it a promising material for investigating hydrogen adsorption and potential hydrogen-storage applications. In this study, MP2 calculations were used to examine H interactions with metal-doped benzene models, which provide simplified representations of graphene's local carbon environment. Among the systems investigated, Li-decorated benzene with H adsorbed on the same side exhibited the most favorable calculated adsorption energy, approximately 0.24 eV, which

falls within the 0.2–0.6 eV/H range frequently discussed in theoretical studies as favorable for reversible hydrogen storage. This result suggests that metal decoration may strengthen H interactions, motivating further investigation of doped carbon materials for hydrogen storage.

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Poster 56:

*Electronic Structure and Magnetism in Predicted Metal-Rich Borides: AlMnRuB, ScMnRuB, and AlReRuB*

**Sneha Panigrahy, Jan. P Scheifers, Boniface P.T. Fokwa**

University of California, Riverside

Rare-earth-free magnetic materials are urgently needed to reduce dependence on critical raw materials in clean energy applications. Metal-rich borides with M:B 2:1 exhibit low-dimensional magnetism from geometrically confined 1D chains of magnetic 3d elements. Three hexagonal borides AlMnRuB, ScMnRuB, and AlReRuB (P62m) predicted within this family satisfy the 105 VE/SBU electronic stability criterion but have never been synthesized or computationally characterized. Spin-polarized DFT calculations were performed using VASP (GGA-PBE, PAW, 450eV, -centered k-mesh, ISYM=1) with NM and FM configurations compared. Chemical bonding was analyzed via pCOHP and ICOHP using LOBSTER. Ferromagnetic ground states are confirmed for AlMnRuB and ScMnRuB, stabilized by 59.2 and 57.7 meV/f.u. respectively. Mn moments of 1.47 and 1.12B form in 1D chains along c, with induced Ru moments ( 0.07 B) confirming 3d-4d hybridization. AlReRuB is non-magnetic. pCOHP analysis identifies removal of Mn-Mn antibonding character at EF as the electronic driving force for FM ordering. B-B dominates structural stabilization via the 1B fragment, while the A-site bond is the strongest interaction at E F . Relaxed lattice parameters for AlReRuB match experimental AlRuB (a=9.31 , c=2.96 ). A-site substitution tunes magnetic electronic structure within a fixed topology - Mn-Sc bonding at E F is stronger than Al-Mn, explaining the reduced moment in ScMnRuB. These results provide the first computational validation of this predicted boride family and motivate future synthesis and magnetic characterization.

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Poster 57:

*Simulating Two-Dimensional Vibrational Spectra with the Data-Driven MB-pol Many-Body Potential*

**Zitong Wu, Richa Rashmi, Eitan Dvorquez, Francesco Paesani**

UCSD

Two-dimensional infrared (2D IR) and IR-Raman (2D IIR) spectroscopies probe couplings among intra- and intermolecular vibrational modes, but simulated 2D spectra are sensitive to the underlying potential energy, dipole, and polarizability surfaces. We combine equilibrium-nonequilibrium molecular dynamics with the data-driven MB-pol potential, trained on CCSD(T) data, and its dipole and polarizability models. Each nonequilibrium trajectory starts from an impulsive kick given by the dipole derivative. For MB-pol, we implement an analytical dipole derivative including geometry-dependent charges and self-consistent induced dipoles under periodic boundary conditions (PBC), solving the induced-dipole equations with particle-mesh Ewald electrostatics. As an application, we compute 2D IIR spectra of high- and low-density supercooled water, comparing MB-pol with q-TIP4P/F, showing distinct signatures of the two liquids.

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Poster 58:

*Enhancing the specificity of biological photosynthesis: Design rules from modeling*

**Shaama M. Sharada, Anya Zoraster**

University of Southern California (USC)

Rising atmospheric CO motivates efforts to improve photosynthetic carbon fixation by ribulose 1,5-bisphosphate carboxylase / oxygenase (Rubisco). Rubisco is responsible for most of carbon fixation but

its efficiency is limited by slow catalysis and competing reactions with O. Our goal is to utilize quantum chemistry methods to probe the mechanism of carbon fixation and identify features that strongly affect activity and specificity. We construct a 160+-atom active-site model of the Rhodospirillum rubrum Rubisco (PDB: 9RUB) enzyme. The model includes Mg, RuBP, one coordinating water, and six residues of which the terminal nitrogen atoms are fixed. All simulations are performed in Q-Chem using the B97X-D/def2-SVP level of theory and the SMD model for implicit solvation. The energetic span model was applied to identify the intermediate and transition state that most strongly influenced the catalytic turnover. Preliminary results suggest that the partial enediol intermediate and the CO addition transition state may be the turnover-determining intermediate and transition state, respectively. Further calculations are needed to complete the pathway and assess whether this assignment remains consistent.

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Poster 59:

*Data-Driven Many-Body Simulations of Biomolecules with CCSD(T) Accuracy: III. A Library of Amino Acid Building Blocks*

**Xinmao Lyu, Ethan Bull-Vulpe, Jiwon Huh, Francesco Paesani**

UC Sandiego

Molecular dynamics simulations of proteins require a potential energy surface that is both accurate and affordable. Conventional force fields rely on a fixed functional form with empirical parameters, whereas machine-learned interatomic potentials (MLIPs) inherit the accuracy of their density functional training data and provide a total energy that cannot be decomposed into physically interpretable contributions. Here, we extend the intramolecular MB-nrg formalism, previously developed for polyalanine, to all 20 natural amino acids. Covalently bonded functional groups are treated as the monomers of a many-body expansion (MBE), short-range 1-, 2-, and 3-body contributions are represented by permutationally invariant polynomials trained on DLPNO-CCSD(T) fragment energies, and all remaining interactions are described by physics-based terms. An automated library decomposes each dipeptide into fragments and samples only previously unseen fragments, using enhanced-sampling simulations and clustering to generate compact training sets. The empirical Lennard-Jones repulsion of our previous model is replaced by a repulsive term derived analytically from exchange-hole dipole moment calculations, so that no parameter is taken from an empirical force field. Assembled from fragment data alone, the resulting potential reproduces the DLPNO-CCSD(T) Ramachandran surfaces of all 20 capped dipeptides with an overall RMSD of 1.26 kcal/mol, compared with 6.65 and 5.43 kcal/mol for Amber ff14SB and ff19SB, which produce systematically too steep surfaces. MLIPs trained on large whole-molecule datasets achieve lower errors on this near-equilibrium, gas-phase benchmark. The largest MB-nrg deviations occur for residues whose side chains interact with the backbone through contributions beyond the 3-body truncation, such as Asn, Gln, and the charged amino acids. Because the MBE makes each contribution explicit, these errors can be traced to their origin: for Asn, adding data-driven non-bonded and 4-body terms reduces the RMSD from 2.15 to 1.08 kcal/mol, provided that the terms are introduced in the order required by the MBE. These results establish a transferable and systematically improvable route toward protein simulations with near coupled-cluster accuracy.

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Poster 60:

*Adding Nuclear Quantum Effects to Mixed Quantum/Classical Models of the Hydrated Electron*

**Talia A. Wagener, William R. Borrelli, Benjamin J. Schwartz**

UCLA

In this work, we investigate how the inclusion of nuclear quantum effects (NQEs) affects the hydrated electron when simulated using two different mixed quantum/classical (MQC) pseudopotentials: TB, which produces a hydrated electron with a hard cavity, and TB-Opt, which produces a softer cavity. We also examine two different water models, SPC/Fw and qSPC/Fw water. By means of path integral

molecular dynamics (PIMD) simulations, we find that NQE's do have a distinct impact on the hydrated electron's solvation shell, and that these structural changes vary with both the pseudopotential and water parameters used. Although bulk SPC/Fw water simulated with NQE's exhibits less structure and faster dynamics than its counterpart with classical nuclei, the effect of including NQE's for water in the hydrated electron's solvation shells is more varied. PIMD simulations of the TB pseudopotential and SPC/Fw water model produce "looser" solvation shells compared to MQC MD with classical nuclei. When the TB-Opt pseudopotential is combined with NQEs however, the degree of local structure increases even though H-bonding seems to weaken. This likely reflects the fact that this particular model has a wider range of first-shell water orientations due to the TB-Opt electrons enhanced fluxionality. The use of qSPC/Fw water simulation parameters similarly influences the hydrated electron's solvation shell in a way that differs from bulk water. With qSPC/Fw and PIMD, the TB electron has a relatively large increase in the rigidity of its first shell, whereas the TB-Opt electron is actually less structured than it is in SPC/Fw water with NQE's. The latter finding, although unexpected, is consistent with the more hydrophobic nature of the TB-Opt electron, which further limits its response to the qSPC/Fw water parameters. Overall, the effect of NQEs on the hydrated electron's solvation structure and dynamics is subtle, and depends heavily on the chosen simulation parameters.

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Poster 61:

*A Systematic Benchmark of Orbital-Optimization Algorithms and Effects of Singly-Singly Mixing in Restricted Open-Shell Kohn-Sham Excited-State Calculations*

**Eugene Kwon, Juan E. Arias-Martinez, Diptarka Hait, and Yuezhi Mao**

San Diego State University and University of California, San Diego

Time-dependent density functional theory (TDDFT) is widely used to calculate molecular excited states, but conventional linear-response formulations can encounter difficulties for charge-transfer characters, states with significant double (or higher) excitation characters, and excitations requiring substantial orbital relaxation. Restricted open-shell Kohn-Sham (ROKS) offers a complementary state-specific approach in which orbitals are explicitly optimized for targeted open-shell singlet excited states. Recent methodological advances have renewed interest in ROKS; however, obtaining reliable ROKS calculations still require careful selection of orbital-optimization algorithms and control over the targeted electronic configuration. Here, we systematically assess the results of ROKS calculations across a chemically diverse set of molecular systems to identify computational settings that reliably converge to the intended excited-state solution while minimizing unintended changes in electronic-state character. We examine the effects of exchange-correlation functional, basis set, self-consistent-field optimization algorithm, and singly-singly orbital mixing on convergence behavior, excitation energies, and electronic-state characters. Particular attention is given to challenging cases prone to partial collapse of the targeted excited state during variational orbital optimization. Our results reveal substantial algorithm-dependent differences in convergence reliability and in the consistency of resultant excited-state energies. Suppressing singly-singly mixing improves the robustness of targeted solutions for several systems examined, reducing unintended changes in excited-state character. These findings provide practical guidance for selecting orbital-optimization algorithms and suggest a strategy for mitigating variational collapse in ROKS calculations. The resulting workflow provides a foundation for more reliable excited-state modeling in photochemical and photophysical applications.

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Poster 62:

*The Role of Proton Transfer in Enzyme-Catalyzed Hydrolysis of Nitriles: A Computational Study of Nit6803*

**Natalia Gelfand, Arieh Warshel**

USC

Nitriles are versatile compounds in organic synthesis because their nitrile group can be converted into various functional groups, including carboxylic acids. However, conventional chemical hydrolysis often requires harsh reaction conditions. Nitrilases offer an alternative by catalyzing the direct conversion of nitriles into carboxylic acids under mild conditions. This direct conversion avoids the formation of amide intermediates. Recent studies have aimed to obtain mutated proteins to better fit particular substrates. A specific substrate, nicotinonitrile, can be converted into nicotinic acid, which is known as vitamin B3 and is an intermediate in the production of various pharmaceuticals. In this work, using computational tools, we aim to investigate how the protein environment can tune catalysis in the nitrilase Nit6803 by controlling proton transfer, which is crucial in the chemical conversion of nitriles. Particular attention is given to the catalytic Glu and Lys residues, whose roles in the enzymatic reaction are still debated.

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Poster 63:

*Spin-Orbit-Driven Polarization in Luminescent Diradicals: From All-Optical Magnetic Field Sensing to a Spin-Resolved Model*

**Ziheng Ma, Jonathan Palmer, Sebastian Kopp, Michael Wasielewski*, Joel Yuen-Zhou***

UCSD

We study non-covalent luminescent diradicals formed by doping TTM radicals into a diamagnetic HTTM host crystal, where adjacent lattice sites yield through-space-coupled triplet pairs confirmed by pulsed EPR. SA-CASSCF/NEVPT2 calculations show that optical spin polarization arises from spin-orbit-driven charge recombination. Fast charge separation (¡500 ps) is followed by recombination that selectively populates the T1 sublevels (SOC = 0.189 vs. 0.002 cm). Unlike covalent TTM diradicals, the SOC is dominated (74%) by one-center chlorine contributions via CT/LE mixing, so crystal packing becomes the design knob. A triplet spin Hamiltonian (—D— = 133 MHz) reproduces the observed magnetoluminescence and enables microwave-free magnetometry at 28 T/Hz, competitive with all-optical NV centers. We also propose a CASSCF-parametrized, spin-resolved essential-state model to predict these observables across crystal geometries.

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Poster 64:

*Stochastic GW with the Orthogonalized Projector Augmented Wave Method*

**Dimitri Bazile, Minh Nguyen, Yuji Kon, Tucker Allen, and Daniel Neuhauser**

UCLA

We introduce stochastic GW with the orthogonalized projector augmented-wave method (OPAW-sGW). This implementation enables accurate quasiparticle band gaps on significantly coarser real-space grids than norm-conserving pseudopotential sGW (NCPP-sGW). The orthogonalized PAW representation preserves the formal all-electron character and enables stochastic sampling of the Greens function and screened Coulomb interaction.

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Poster 65:

*Big Teacher, Small Student: Tackling the Accuracy-Speed Trade-Off of Permutationally Invariant Polynomials*

**Elijah Garcia, Xinmao Lyu, Francesco Paesani**
UC San Diego

Permutationally Invariant Polynomials (PIPs) are a proven method for creating highly accurate and improvable potential energy surfaces, most famously used in a many-body expansion framework. For this type of potential, the accuracy of the model (with sufficient training data) is directly correlated with the size of the model. With existing PIP fitting strategies, a more accurate model will by construction be a larger and slower model.

For a fragmented CONH-CH-CONH system, a teacher model was created with a delta-learning approach. A 76,075-term PIP was first fitted to 51,259 UMA data points. A 2,925-term PIP and Gaussian-process correction was then fitted to the difference between the first model and the DLPNO-CCSD(T) energies for 3,668 structures. The combined teacher model was then used to create a synthetic dataset of energies and forces. The student model, a single PIP, was subsequently trained on this synthetic dataset. Once trained, PIP terms were systematically removed from the model to reduce its size.

A 20,863-term student model with no Gaussian-process correction was created with only a 3% increase in test-set error compared to the teacher, while evaluating 7.8x faster than the teacher model. At an intermediate size, a 4,000-term student model achieved a 40x speed-up compared to the teacher with a test-set error of 0.10 kcal/mol (2.9% of the total spread). In the most extreme case considered, a 1,000-term model was prepared with a test error of 0.150 kcal/mol and a 154× speed-up. The forces of this model differ from the teacher's by 0.81 kcal/mol/, suggesting it is too inaccurate for reliable dynamics.

This framework for preparing PIPs greatly increases their evaluation speed while retaining nearly the same accuracy. It also allows the option of extremely fast models that intentionally sacrifice accuracy if desired. Further research will test this approach on other systems to ensure its robustness.

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Poster 66:

*Investigating the Effects of Lysine Acetylation on PTBP1 Structural Dynamics Through Molecular Dynamics Simulations*

**Donald Chang, Francesca Bautista, Niroshika Keppetipola Ph.D, Kenneth Childers Ph.D**
CSU Fullerton

Alternative splicing is an essential mechanism of gene regulation that contributes to protein diversity, with aberrant splicing patterns implicated in the progression of cancers, including breast and colon cancers. Polypyrimidine tract-binding protein 1 (PTBP1) is an RNA-binding protein containing four RNA recognition motifs (RRMs) that regulates alternative splicing through interactions with pre-mRNA transcripts. Post-translational modifications, such as lysine acetylation, can alter the physicochemical properties of proteins by neutralizing positively charged lysine residues, potentially affecting electrostatic interactions, hydrogen bonding, and conformational dynamics. Although lysine acetylation has previously been identified within PTBP1, its structural effects remain poorly understood. This study employs molecular dynamics (MD) simulations to investigate how site-specific lysine acetylation influences PTBP1 conformational behavior and evaluates the accuracy of amino acid substitutions commonly used to mimic acetylated and non-acetylated states. Using an NMR solution structure of PTBP1 RRM3-RRM4, previously identified acetylation sites within RRM3, RRM4, or both domains were modified with acetylation-mimic glutamine (KQ), deacetylation-mimic arginine (KR), or acetylated lysine (AcK). Modified structures were compared to the deacetylated wild type. GROMACS MD simulations were conducted at 500 ns per system, with and without RNA. Structural dynamics were

evaluated through root-mean-square deviation (RMSD), root-mean-square fluctuation (RMSF), radius of gyration (Rg), and hydrogen-bond analyses. Preliminary analyses indicate that lysine modifications influence the conformational dynamics and protein-RNA interactions of PTBP1 RRM3-RRM4. For RNA-bound systems modified within both domains, glutamine-substituted PTBP1 exhibited increased conformational fluctuations and a larger radius of gyration, with an average Rg of 1.870 nm and RMSF of 0.286 nm, compared to 1.817 nm and 0.224 nm for wild type, respectively. Arginine-substituted PTBP1 maintained a mean Rg comparable to wild type (1.815 nm), whereas explicitly acetylated PTBP1 exhibited a lower average RMSF (0.219 nm) despite a higher mean Rg (1.858 nm). Protein-RNA hydrogen-bond analysis revealed higher average hydrogen-bond counts for wild-type (13.98) and arginine-substituted (12.72) systems compared to glutamine-substituted (5.79) and explicitly acetylated (7.17) systems. These differences suggest that lysine modifications may influence the organization of protein-RNA interactions, potentially through changes in side-chain chemistry and local conformational dynamics. Differences in conformational fluctuations and protein-RNA hydrogen bonding between glutamine-substituted and explicitly acetylated systems suggest that KQ substitutions may not fully reproduce the structural and interaction dynamics associated with lysine acetylation. Substantial RMSD changes in both glutamine-substituted and wild-type systems highlight the need for additional sampling and independent replicates to assess conformational convergence.

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Poster 67:

*Minimum energy crossing accessibility, internal conversion rates, and the fluorescence turn-on effect in DEA-tC*

**Harrison Pearce, Byron W. Purse, Andrew L. Cooksy**

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8-Diethylamino-tricyclic-cytosine (DEA-tC) is up to 20 times more fluorescent when base-paired with guanine in double-stranded DNA (dsDNA) than when it is a free nucleoside. DEA-tC is relatively non-emissive as a nucleobase, with a fluorescence quantum yield of 0.006. The change from being non-emissive to emissive upon base pairing is desired in fluorescence turn-on sensing, and its similarity to cytosine minimizes structural perturbation upon incorporation into DNA and RNA. Unfortunately, DEA-tC is relatively cytotoxic, unlike other tricyclic cytosine analogs, and it isnt metabolized, unlike the other tricyclic cytosine analogs. A recent base pairing study indicates that tautomerism may be the cause for the fluorescence turn-on effect on DEA-tC. In this hypothesis, a cytosine like tautomer (C-like) is relatively bright compared to a thymine like tautomer (T-like), and base pairing with guanine stabilizes the C-like tautomer. In this work TD-DFT methods are used to test the effects of tautomerism, hydrogen bonding, and base pairing on the accessibility of minimum energy crossing points (MECPs) between the S1 and S0 electronic potential energy surfaces. Internal conversion (IC) rates in the weak coupling regime are also calculated in the same systems with an adiabatic hessian (AH) model and nonadiabatic couplings. tC. Although MECPs aren't accessible without a shift in energy, qualitative trends in MECP accessibility agree with known experimental trends in fluorescence quantum yield, which support a relative dim T-like tautomer and bright C-like tautomer. The calculated IC rates dropped significantly when base paired. This trend was intensified in tricyclic cytosine, a tC analog which experimentally doesn't have a pronounced turn-on effect, indicating that, while the rate of IC is reduced upon base pairing, this is not the cause of DEA-tC's unique turn-on effect.

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Poster 68:

*Circumventing Hyperpolarization in NMR*

**Natalia Munoz-Barraza, Arghadip Koner, Joel Yuen-Zhou**

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The inherently low sensitivity of nuclear magnetic resonance (NMR) spectroscopy has motivated numerous hyperpolarization techniques that enhance signals by generating nonequilibrium nuclear-spin populations. Depending on the technique, requirements such as chemical additives, specific substrate chemistry, or cryogenic preparation can limit their applicability. Here, we theoretically investigate an alternative protocol based on probing a sample at room temperature with single-photon states and measuring changes in the photon-number statistics before and after the sample. We compare these results with those obtained using coherent-state probes at low and high mean photon numbers. In the regimes examined, single-photon Fock states produce larger changes in these photon-number probabilities, suggesting a potential advantage and motivating further investigation of quantum light as a resource for NMR detection.

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Poster 69:

*ELFnet: Predicting Electron Localization Functions from Superposed Atomic Densities for Accelerated Superhydride Discovery*

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The electron localization function (ELF) reveals chemical bonding and interstitial electron localization, but calculating three-dimensional ELF fields with density functional theory (DFT) is costly for large-scale materials screening. We present ELFNet, a deep-learning model that predicts DFT-derived ELF fields from inexpensive superposed atomic density (SAD) inputs, enabling rapid screening of chemical templates under pressure. The training dataset contains 326,009 converged unary and binary prototype structures spanning 89 elements and pressures of approximately 50 to 500 GPa, calculated using the Perdew-Burke-Ernzerhof functional. ELFNet combines periodic full-grid convolutions with a composite loss function designed to capture sparse regions of strong electron localization. Evaluation on 50,000 metal-only templates derived from known high-pressure superhydride prototypes shows that the predicted fields reproduce chemically meaningful differences in the spatial arrangement of interstitial localization. Maximum ELF values and the positions of these maxima provide complementary measures of agreement with DFT. On the tested hardware, the complete prediction and file-writing workflow reduced summed per-structure elapsed time by approximately 350-fold compared with fixed-geometry VASP ELF calculations. ELFNet therefore offers an efficient initial screening tool for identifying promising metal templates for subsequent first-principles validation.

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Poster 70:

*An Effective Machine Learning Frame for Materials Discovery Structured by a Chemical Concept*

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Machine learning can accelerate materials discovery, but exploring complex crystal structures remains challenging because of the vast number of possible atomic arrangements. We present a machine-learning workflow guided by chemical template theory that simplifies this search by first identifying promising metal frameworks. The theory describes how electron localization in the interstitial regions of a metal lattice creates a chemical template that stabilizes an associated nonmetal network. Using high-pressure

superhydrides as a test system, we translate this principle into a two-stage discovery strategy: machine learning screens metal templates, and targeted crystal structure searches determine hydrogen arrangements within the selected frameworks. A stacked ensemble model is trained on 4,151 structures using 46 descriptors of metal identity, lattice geometry, composition, and interstitial electron localization. The model predicts thermodynamic stability without requiring the detailed hydrogen arrangement, achieving a cross-validation mean absolute error of 11 meV/atom and R of 0.951. The maximum and average interstitial electron localization functions rank among the most influential descriptors, supporting the physical basis of the approach. Screening 7,939 candidate metal lattices identifies 1,421 promising templates for subsequent structure searches and first-principles validation. This workflow yields 31 predicted stable superhydrides spanning 13 new structural prototypes, including complex structures with non-integer hydrogen-to-metal ratios and up to 94 atoms per primitive cell. These results demonstrate how chemical theory can guide both feature selection and the organization of a machine-learning workflow, reducing the structural search space and enabling systematic discovery of complex materials.

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Poster 71:

*Chemical templates that assemble the metal superhydrides*

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Understanding how electrons organize between atoms offers a route to explaining crystal structures and guiding materials discovery. Quasi-atom theory extends the conventional atom-centered description of bonding by introducing local electronic orbitals centered in interstitial regions without nuclei. Electrons occupying these orbitals can behave as anions or participate in bonding with neighboring atoms and other quasi-atoms. This framework has explained the formation of high-pressure electrides, the emergence of bonded quasi-molecules and semiconducting behavior in compressed lithium, and systematic trends in elemental metal structures across the periodic table, including transitions to complex structures under pressure.

Chemical template theory builds on this foundation to explain how metal sublattices stabilize complex compounds. Even when a metal is not a conventional electride, partial occupation of its interstitial quasi-atom orbitals can produce a spatial pattern of electron localization that acts as a chemical template. The strength and geometry of this template depend on metal identity, lattice structure, and compression. In metal superhydrides, the interstitial orbitals of the metal framework match the electronic states of the hydrogen network, stabilizing its three-dimensional aromatic building units and promoting the formation of extended H-H bonding networks. High-throughput first-principles calculations and model-system analyses show why metals near the s-d boundary form particularly effective templates and explain structural preferences that cannot be accounted for by direct metalhydrogen bonding or charge transfer alone.

Beyond explaining known materials, chemical template theory provides a practical strategy for discovering new structures: first identify metal frameworks with suitable interstitial electron localization, then search for compatible nonmetal arrangements within those frameworks. Applications to binary and ternary superhydrides demonstrate that this approach can substantially accelerate structure searches and reveal previously unexplored compositions. The same principle provides physically motivated descriptors and a two-stage architecture for machine-learning-assisted discovery, linking fundamental elec-

tronic structure to efficient exploration of complex chemical spaces.

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