	First name	Last name	Intstitute	Title of your presentation/ poster	Abstract of your presentation/poster (250 words)
1	Matt	Wellborn	Caltech	TBA	TBA
2	Ioan	Magdau	Caltech	2D THz-THz-Raman Spectroscopy from MD: Bromoform	
3	Zhendong	Li	Caltech	Towards Understanding Electronic Structures of Iron-Sulfur Clusters by DMRG and Spin Projections	Polymetallic transition metal compounds such as iron-sulfur clusters in biology have fascinating chemical and physical properties due to the large number of unpaired d electrons. However, such systems are beyond the scope of the density functional theory (DFT) due to the strong correlation among different transition metal centers. The density matrix renormalization group (DMRG) is a powerful tool for strongly correlated systems. For iron-sulfur clusters, two problems need to be addressed: 1. Different spin states need to be resolved. 2. Local minimums are to be avoided. In this work, we present an approach named spin-projected matrix product states (SP-MPS) to tackle these problems.
4	Michiel	Niesen	Caltech		
5	Victor	Fung	UCR	Exploring Structural Diversity and Fluxionality of Pt_n (n = 10–13) Clusters from First-Principles	Subnanometer transition-metal clusters have been shown to possess catalytic activity that is size-dependent. It has been suggested that the fluxionality of these small clusters may be closely related to their catalytic activity. Here we use basin-hopping global optimization with density functional theory (DFT) to study the energy landscape of Pt_n (n = 10–13) clusters. We analyze a large set of local minima obtained from the DFT-based global optimization. We find that Pt_{10} is unique with respect to the other studied sizes in its structural landscape, which shows a single, distinct structural motif corresponding to a tetrahedral global minimum. In contrast, Pt_{11-13} all display characteristics of high fluxionality with the presence of multiple significantly differing structural features in the low-energy region, as characterized by coordination number, interatomic distances, and shape. These observations demonstrate the structural diversity and fluxionality of the subnanometer Pt clusters that will have important implications for catalysis.
6	Peter	Langhoff	UCSD	Quantum-Mechanical Definition of Atoms and their Interactions in Molecules	In the apparent absence of meaningful assignments of electrons and indistinguishable nuclei to particular atoms in molecules, the electronic energies of individual constituent atoms and the bonding or non-bonding interaction energies between them are widely perceived as fundamentally undefined in molecular quantum theory. Additional conditions are accordingly required to achieve specificity, giving rise to many subjective individual definitions. Here we resolve the issue of assignments of electrons to atoms within molecules at the Born-Oppenheimer level of theory, and provide objective quantum-mechanical definitions of atomic operators and of the interaction potentials between them. A van-der-Waals subgroup of the full molecular electronic symmetric group is shown to facilitate assignments of electrons and indistinguishable nuclei to particular atoms in a molecule. Self-adjoint atomic and atomic-interaction operators defined in this way are seen to have Hermitian matrix representatives and physically significant expectation values in totally antisymmetric molecular eigenstates. Electronic molecular energies emerge naturally from the development in the form of sums of energies of the individual atomic constituents and of their atomic pairwise interactions in the absence of subjective auxiliary conditions. A detailed and nuanced description of electronic structure and bonding is provided thereby which includes the interplay between atomic promotion and interaction energies, common representation of atomic-state hybridization and inter-atomic charge apportionment, and measurable atomic-state entanglements upon coherent dissociations of polyatomic molecules. The related question of quantum-mechanical definition of the geometrical structures of molecules in the absence of the classical fixed-nuclei Born-Oppenheimer approximation is indicated in an extension of the formalism.
7	Jorge	Campos Gonzalez Angulo	UCSD	Coarse simulation of the dynamics of an auxetic, two-dimensional protein crystal.	In this work, we present the dynamical behavior of a 2D lattice obtained by the tessellation of the C4-symmetric protein L-rhamnulose-1-phosphate aldolase (RhuA). From a purely geometric point of view, we analyze the symmetries exhibited by the lattice, and their repercussion on the degrees of freedom required to describe such behavior. Molecular dynamics calculations on these degrees of freedom provide essential information towards the understanding of the coherent behavior observed experimentally.

8	Luis Angel	Martinez-Martinez	UCSD	Polariton-assisted singlet fission	Singlet-fission is a process in which a singlet excitation in a molecular ensemble undergoes fission into two triplet excited states. This phenomenon has attracted the attention of the scientific community as a means to significantly increase the efficiency of organic photovoltaic devices. On the other hand, with the advent of highly confined structures in recent years, it has been possible to achieve a Strong Coupling (SC) light-matter regime. Under this regime, recent works have shown the emergence of new phenomena related to the photonic dressing of the molecular states, for instance, tuning of chemical reactivity and exciton transport. In this work, we explore the implications of SC on singlet fission kinetics and the relevance of polaritonic states in the coupling between the singlet and triplet-triplet excited manifold of a model molecular ensemble.
9	Francisca	Sagredo	UCI	Exact and approximate ensemble density functionals for a model system	
10	Daniel	Sheehan	USD	Superdegeneracy and thermally-mediated population inversion	Population inversion (e.g., in lasers) is a nonequilibrium phenomenon owing to the dominance of the Boltzmann factor in determining state occupancy under thermal equilibrium. State degeneracy, while adding detail, is assumed to be of secondary importance. In this poster, special circumstances are considered under which degeneracy dominates the Boltzmann exponential, leading to population inversion at thermal equilibrium. Physical systems that might exhibit this anomalous degeneracy effect are proposed and possible applications are discussed..
11	Sarah	Allec	UCR	GPU-Enabled Real-Time Electron Dynamics of Nitrogen-Doped Graphene Nanoflakes	Since its isolation in 2004, graphene has become one of the most promising materials of the twenty-first century, particularly for next-generation electronics. Because conventional silicon-based electronics face fundamental limitations at the nanoscale, preparing graphene for use in carbon-based nanoelectronics has been the focus of intense research. One of the most powerful and feasible methods of tailoring the properties of graphene is by doping with foreign atoms. Nitrogen, with a similar size to carbon but with one more electron, is expected to form donor states in graphene as a substitutional dopant; however, experimental measurements of N-doped graphene reveal the existence of several nitrogen configurations with distinct electronic properties. In particular, one can tune the charge carrier concentrations by controlling these dopant bonding configurations to transform graphene into a p-type or n-type semiconductor. While there have been previous experimental and theoretical results for nitrogen-doped graphene, there has not been a systematic study of these materials at the nanoscale, where optoelectronic properties are heavily governed by quantum confinement effects. To this end, we have carried out a theoretical investigation of nitrogen-doped graphene nanoflakes via a new real-time time-dependent density functional tight binding (RT-TDDFTB) code that runs on massively-parallelized GPUs. This GPU-enhanced capability allows us to efficiently and accurately calculate the electron dynamics of these systems (~1400 atoms), whereas conventional approaches are computationally limited to hundreds of atoms. Our use of high-performance GPUs permits an efficient approach for understanding the effects of graphene dopants to rationally guide experimental efforts in harnessing these novel materials.
12	Sebastian	Lee	Caltech	TBA	TBA

13	Daniel	Moberg	UCSD	Molecular Origin of the Vibrational Spectrum of Ice Ih in the OH Stretching Region	Despite more than 50 years having passed since the first measurements of the vibrational spectra of ice Ih, an unambiguous assignment of the different features observed in the infrared (IR) and Raman spectra remains a matter of debate. This study demonstrates that the application of many-body molecular dynamics (MB-MD), which enables simulations of water with chemical and spectroscopic accuracy from the gas to the condensed phase, leads to a unified interpretation of the vibrational spectra of ice Ih in terms of the underlying molecular structure and dynamics. In particular, it is shown that all peaks of the IR and Raman spectra in the OH stretching region can be unambiguously assigned by taking into account both the symmetry and the delocalized nature of the lattice vibrations as well as the local electrostatic environment experienced by the water molecules within the crystal. The unprecedented accuracy of the simulations presented here indicates that quantum MB-MD can enable predictive studies of ice which, complementing analogous experimental measurements, can provide molecular-level insights into fundamental physicochemical processes taking place in bulk ice and on ice surfaces.
14	Sheng	Guo	Caltech		
15	Pavel	Pokhilko	USC	Spin-forbidden channels in reactions of unsaturated hydrocarbons with oxygen	From the previous experimental and theoretical works it is known that in the reaction of ethylene and O(3P) not only the lowest triplet surface contributes to the products and branching ratios, but also the singlet surface. In order to understand the influence of other states, we have considered 4 lowest electronic states of the CH2CH2O and CHCHO intermediates in the reactions of ethylene and O(3P), and acetylene and O(3P) respectively. We found that these intermediates are chemically different from each other. CH2CH2O has a single C-C bond, allowing CH2 group to rotate almost freely on the lowest triplet surface, causing intersystem crossing of the lowest singlet and triplet states. CHCHO has a C-C bond of double character, which constrains rotation along the bond and forms E- and Z-isomers. Spin-orbit coupling constants (SOCCs) of these states are extremely sensitive to the nature of states: SOCCs are different by two orders of magnitude, e.g., 0.43, 10.86, 58.15 cm -1 for one of the geometries of CH2CH2O. This difference can be explained by extension of El-Sayed rule to Natural Transition Orbitals. We analyzed performance of different methods in EOM-CC family and concluded that balanced description of all states in the manifold is crucial.
16	Marc	Riera Riambau	UCSD	Toward Chemical Accuracy in the Description of IonWater Interactions through Many-Body Representations	Electrolyte solutions play an important role in many natural and industrial processes, ranging from those that take place inside living cells, in marine environments, on atmospheric aerosol particles, and at electrochemical interfaces. In order to understand all these processes, an accurate molecular level description is needed. In this work, new potential energy functions in a classical framework (i-TTM) and a quantum-mechanical framework (mb-nrg) for alkali-water and halide-water systems are presented. These potentials are derived from fits to highly accurate electronic structure calculations (CCSD(T) with TQ extrapolation) and include an explicit treatment of the two body repulsion, electrostatics, and dispersion energy. The many body effects are recovered through classical polarization within an extended Tholetype model. The accuracy of these potentials will be assessed through the analysis of the interaction and binding energy of ion-water clusters in the gas phase, which will be compared with the ones obtained with CCSD(T) and DF-MP2 for optimized structures at the DF-MP2 level of theory, and comparison of harmonic and anharmonic frequencies obtained with I-TTM and mb-nrg with experiments and frequencies from coupled cluster. The accuracy of these two sets of potential energy functions will be also compared with some common methodologies used in the scientific community such as DFT and classical force fields like AMOEBA.
17	Devon	Widmer	UCLA	Condensed Phase Dynamics of the Sodium Dimer Cation	

18	Victoria	Lim	UCI	Molecular modeling of small molecule inhibitors of the Hv1 proton channel	Hv1 is a voltage-sensitive proton channel whose main function is to extrude acid from cells. It is the most selective ion channel known and appears to be involved in a wide variety of maladies (e.g., autoimmune diseases, atherosclerosis, brain damage in ischemic stroke). Despite extensive recent research, details of the gating mechanism, proton permeation pathway, and exquisite selectivity of Hv1 remain elusive. We have previously developed an atomistic model of human Hv1 in its open state using molecular dynamics (MD) simulations in the 10 μs timescale. This model has been validated by comparison with electrophysiology data. Further investigation of the model with respect to small molecule inhibitor binding may further validate the structure and lead to the design and development of effective channel blockers. The objective of this work is to understand and improve the binding of small molecules that have been experimentally shown to block Hv1. Our approach utilizes the docking of these inhibitors to our open state model, atomistic molecular dynamics simulations, and alchemical free energy calculations. Here, we present preliminary results on the relative binding free energies of these Hv1 inhibitors with comparison to experimental mutagenesis and electrophysiology data.
19	Niranjan	Ilawe	UCR	Plasmonic Resonances: A Systematic Analysis of Metallic Nanoparticles Using Real-Time, Time-Dependent DFTB	Recent advances in the study of local surface plasmon resonances (LSPRs) in metallic nanoparticles (NPs) have led to the emergence of novel applications in chemical and biological sensing, nanophotonic devices, and energy harvesting. Crucial to the advancement of these applications is a predictive, theoretical understanding of LSPRs with regard to NP shape, size, composition, and environment. Classical electrodynamic theories, based on solving Maxwell's equations, frequently used to investigate the optical properties of metal NPs, fail to account for the atomistic details and quantum effects. On the other hand, ab-initio quantum mechanical calculations such as density functional theory, while accounting for quantum properties are computationally costly and currently limited to very small NPs. In this poster, I will describe my use of the density functional tight-binding (DFTB) approach and its real-time time-dependent counterpart, RT-TDDFTB, to probe the excited-state dynamics of large plasmonic nanostructures. Specifically in my poster presentation, I will discuss the results obtained by the RT-TDDFTB calculations, applied to (1) study the shape and size dependence of LSPR energy of large sodium NPs (up to 7nm, containing about 2800 atoms) (2) the electric field enhancement calculations, which display "hot spots" on regions of highest local curvature (i.e., at the corners of the structure) and (3) computational results analyzing effect of surface oxidation on LSPR energy corroborating experimental findings. In summary, my poster will demonstrate the use of RT-TDDFTB calculations to provide an intuitive approach to probe in atomistic detail the real-time electron dynamics in large plasmonic NPs.
20	Zied	Gaieb	UCSD	D3R Grand Challenge 2: Blind Prediction of protein-ligand poses, affinity rankings, and relative binding free energies	The Drug Design Data Resource (D3R) aims to advance the technology of computer aided drug discovery (CADD) by holding community-wide, blinded prediction challenges that rigorously test various docking, scoring, and free energy methods against high quality experimental data. D3R's second Grand Challenge (GC2) was based on the Farnesoid X Receptor (FXR) and comprised 36 co-crystal structures and 102 IC50s. Among the 102 compounds, 96 belonged to four different chemical series (benzimidazoles, isoxazoles, spiros and sulfonamides), and six were classified as miscellaneous compounds. As with Grand Challenge 2015, GC2 involved two stages. In stage 1, participants could submit pose predictions of the 36 ligands with available co-crystal structures, potency rankings of all 102 ligands, and calculations of relative binding affinities within two subsets of 15 sulfonamides and 18 spiros by alchemical methods. In stage 2, available co-crystal structures were made publicly available and participants were to repeat the affinity predictions or rankings and relative binding affinities using the additional disclosed information. Over 250 prediction sets were submitted from nearly 50 participants. The accuracy of participant submissions was evaluated using a variety of metrics which included the symmetry-corrected root-mean-square deviation (RMSD) of predicted versus crystallographic poses, rank correlation coefficients (Kendall's tau and Spearman's rho), and a centered root-mean-square error (RMSEc). This presentation will evaluate the results across all submitted predictions and draw broad conclusions on the performance of the varied methods. The Continuous Evaluation of Ligand Pose Prediction (CELPP) challenge and a roadmap of future grand challenges will also be briefly presented.

21	Caitlin	Bannan	UCI	Improving Force Field Parameterization with Bayesian Inference for Chemical Perception	We are developing a Bayesian approach for creating molecular modeling force fields. These force fields are used in a variety of research fields including computer-aided drug design, biomaterials, and polymer chemistry. Yet, there are many problems that need to be addressed to improve force fields and make them easier to create. Current parameterization of these force fields requires years of human effort and depends heavily on the chemical intuition of experts involved. We will replace this tedious process with an automated machinery to learn parameters and chemical perception. In most common force fields, atomtypes describe chemical perception by classifying atoms based their environment. Traditionally, atomtypes are hand picked by the scientists and then parameters are fit to experimental and quantum data for each combination of atomtypes. Our new format, SMIRKS Native Open Force Field (SMIRNOFF), allows all parameter types to be defined independently, reducing the redundancy resulting from atomtypes. We introduce a tool called SMIRKY that is able to discover chemical perception for a variety parameter types from reference data using a Reversible Jump Markov Chain Monte Carlo algorithm. Here, we will showcase results from testing SMIRKY on a variety of molecule sets. This technique combined with Bayesian inference methods to learn parameters will ultimately be used to generate a SMIRNOFF from reference data. This automated machinery will allow tests of which functional forms are able to be best fit a particular set of input data and be most predictive, without testing the skill of the person doing the parameterization.
22	Elena	Arroyo	San Diego state	Mucus Model	Mucus networks have recently garnered attention in their potential to aid phages in their search for bacterial hosts. Despite this, the complex interactions between the mucus, phages, and bacteria are still largely unexplored. Several possible mechanisms by which mucus could aid phages are (1) phages stick to mucus, thereby increasing the encounter rate with bacteria (2) bacteria influence the viscoelastic properties of a mucus network making it easier for phages to move towards them. A large-scale parallel computer simulation of a mucus network that we are currently developing will be discussed. In this model mucins contain three different types of groups: polar (P), hydrophopic (H), and sulfide (S). Several properties of the mucus network will be shown and compared with experimental data. For example, the radial distribution function of the H and S groups and the lifetimes of the HH and SS bonds that these groups form. In the future, we plan to use this code to study the mucus, phage, and bacteria interactions.
23	Alexander	Sokolov	Caltech	Time-dependent Multi-Reference Perturbation Theory for Strongly Correlated Systems	I will describe a new method which provides an efficient description of static and dynamic electron correlation by combining the formalism of density matrix renormalization group (DMRG) and time-dependent multi-reference perturbation theory. This approach has a number of important advantages: 1) It is equivalent to fully uncontracted perturbation theory, but has a lower computational scaling than the contracted approaches; 2) It avoids computation of the three- and four-particle reduced density matrices; 3) It has a polynomial scaling with the number of active orbitals and can be applied to active spaces with much more than 24 orbitals. I will present a brief overview of multi-reference time-dependent perturbation theory, discuss its implementation in combination with DMRG, and demonstrate its performance for strongly correlated systems with large active spaces.
24	Mai-Anh	Ha	UCLA	Borated Pt Subnanoclusters on Metal Oxides: Coke prevention via minimizing dehydrogenation of alkenes and C-sticking	We present a realistic ab-initio study of subnanoclusters considering the ensemble effects of relevant minima on chemical stability against coking and reactivity to possible dopants in conjunction with experiment. Clusters supported on α-alumina (0001) and MgO (100) share similar bonding trends such as a B-O anchor to the support and decreased charge transfer from the metal oxide to the cluster. While clusters on MgO are dominated by a single minimum, those on α-alumina contain many local minima, which present a mix of dimensionality influencing catalysis. For clusters on alumina, temperature programed desorption (TPD) mass spectrometry identified dehydrogenation trends of both ethylene (as a precursor to coke) and diborane (the borating reagent to Pt) in the cluster range of n = 4, 7, and 8, while theory examined the electronic structure on chemical stability and reactivity. Two pathways to circumvent coking were explored: minimizing the dehydrogenation of alkenes and carbon sticking energies. The coverage dependence of alkene adsorption and coking of minima, composed of >99% of Boltzmann populations at relevant temperatures of 450 and 700 K, provided an approximation of catalytic conditions. Moreover, we answer the question of the effectiveness of the borating agent, diborane, as a dopant as well as the influence of borated Pt catalysts on coke prevention.

25	Chris	Lee	UCSD	Investigating transport properties with multiscale computable mesh models from heterogeneous structural datasets	Individual modeling techniques are often applicable in limited spatial-temporal domains leading to gaps in our biological modeling capabilities. To bridge these gaps, new methodological solutions to integrate levels of resolution are necessary. Mesh models can represent spatial data across all size scales, furthermore, they can be used with various levels of simulation resolution. Thus mesh structures provide an ideal integrative platform for multiscale modeling. In this work, we describe a workflow to convert structural datasets, such as those from electron microscopy or x-ray crystallography, into mesh models suitable for modeling. To ensure that resultant meshes are ``compute quality'' we employ a redesigned version of GAMer (Geometry-preserving Adaptive MeshER), a mesh generation tool that produces and refines high-quality simplex meshes. GAMer is available as a stand-alone package or it can be accessed as a plug-in to 3D-modeling software Blender. To improve the robustness of mesh generation, we have implemented automated detection and resolution of many common mesh defects. Drastic improvements in structural biology methods have lead to an abundance of structural datasets ranging from protein structures to subcellular images. The development of an integrative multiscale meshing platform can yield important new biological insight into the effects of physiology and anatomy on function. These multi-scale models will provide new opportunities for drug discovery and have an impact on human health and longevity.
26	Giulia	Palermo	UCSD	CRISPR-CAS9: COMPUTATIONAL INSIGHTS TOWARD IMPROVED GENOME EDITING	Life sciences are undergoing a transformative phase due to an emerging genome-editing technology based on the RNA-programmable CRISPR-Cas9 (clustered regularly interspaced short palindromic repeats-CRISPR associated protein 9) system. Cas9 is an RNA-guided endonuclease that cleaves double stranded DNA, while forming an RNA:DNA hybrid and a displaced non-target DNA strand. Although extensive structural studies are ongoing, the conformational dynamics of the endonuclease Cas9 and its interplay with the nucleic acids during association and DNA cleavage are largely unclear. This missing aspect hampers the precise structure-based design of CRISPR-Cas9 genome-editing tools with improved specificity. Here, we report the first biophysical study – based on extensive multi-microseconds molecular simulations integrated with structural data – revealing the conformational plasticity of Cas9 and identifying the key determinants that allow its large-scale conformational changes during nucleic acid binding and processing. We identify a remarkable conformational plasticity as an intrinsic property of the nuclease HNH domain, being a necessary factor allowing for the HNH domain repositioning during catalysis. More importantly, we disclose a key role of the non-target DNA during the process of activation of the HNH domain, showing how the non-target DNA positioning triggers local conformational changes that favor the formation of a catalytically competent Cas9. Our outcomes further suggest new and precise protein-engineering modifications, which are of fundamental importance for the rational design of more effective genome-editing tools. Overall, these novel findings constitute a reference for future experimental studies aimed at a full characterization of the dynamic features and at the improvement of biological applications of the CRISPR-Cas9 system.
27	Joshua	Kretchmer	Caltech	Non-equilibrium electron dynamics from real-time active space methods	The simulation of real-time electron dynamic in correlated systems, such as in molecular junctions, molecular wires, and photoexcited materials, provides a challenge for theoretical methods. Towards this goal, we introduce and compare a real-time extension of the density matrix embedding theory (DMET) to time-dependent complete active space self-consistent field (TD-CASSCF) theory for the simulation of real-time electron dynamics in strongly correlated systems. As in the previously developed static DMET, real-time DMET partitions the system into a subsystem, corresponding to the region of interest, coupled to the surrounding environment, which is efficiently represented by a small quantum bath. The accuracy of both real-time DMET and TD-CASSCF is investigated through comparison to numerically exact results for a range of quantum quenches in the Anderson impurity model, a model system for strongly correlated electron dynamics. Furthermore, real-time DMET and TD-CASSCF are able to simulate system sizes beyond those that can be treated numerically exactly, allowing for convergence towards the, previously unobtainable, thermodynamic limit.

28	Thomas E.	Baker	UCI	Approximating Natural Orbitals with a Product Plane Wave Basis	Natural orbitals are known to be effective basis sets for a given problem. They converge very quickly to the ground state energy with the number of functions used. However, obtaining the natural orbitals requires a full, expensive solution of the fully interacting Hamiltonian. A product plane wave ansatz is developed to simulate the natural orbitals without solving the interacting problem. We expand a Jastrow function in terms of trigonometric functions based on an orbital from the relatively cheap local density approximation, though another approximate theory can be used. Within a few functions, the basis is convergent and provides the ground state energy. We test this ansatz in one dimension and discuss generalizations to three dimensions.
29	Moises	Romero	CSUSB CREST	A Computational Outlook on Ferroelectricity: Transition State Optimizations and Charge Analysis	Croconic acid and 1,4-diazabicyclo[2.2.2]octane (DABCO) are strong organic ferroelectrics due to their high spontaneous polarization; however, DABCO's ferroelectric activity is only viewed in certain cocrystals. Both crystal structures' ferroelectric activity is related to their proton transfer mechanism. Prior studies on croconic acid's proton transfer transition states have been performed, however the theoretical calculations found only one possible lowest energy maxima with the method used. This study seeks to reuse the interpolation method from the prior studies as well using the nudge elastic band method (NEB) which is a better predictor for the lowest energy maxima. Results for DABCO showed the interpolation method having an energy barrier of .32eV; however the NEB method predicted two images of which had an energy barrier of .26eV and .24eV. Results for croconic acid for the interpolation method showed an energy barrier of 1.15eV and NEB method an energy barrier of .56eV. Charge density difference and polarizations were also calculated.
30	Bryan	Herrera	Western Universiy	Molecular Dynamics and Virtual Screening of Pituitary Adenylyl Cyclase Type I Receptor Antagonists	The pituitary adenylyl cyclase type I (PAC1R) is a class B G-protein coupled receptor, which mediates the action of pituitary adenylyl cyclase activating polypeptide (PACAP). This peptide/receptor system is known to be involved in neuronal survival and tumorigenesis. However, the lack of available small-molecule ligands that bind to PAC1R and are systemically bioavailable limits pharmacological investigations regarding the importance of this PACAP/PAC1 receptor system. In an attempt to better understand the role of this system in pathophysiological responses, we derived selective antagonists through molecular dynamics (MD) simulations and virtual screening. Peptide segments were designed based on a contact map analysis using trajectory data over a 4 replicate, 100 nanosecond molecular dynamic simulation of the PAC1R ectodomain bound with PACAP. The designed peptide segments were simulated with an identical system to determine the binding stability and serve as starting point for peptidomimetics design. In addition, the most frequent conformations of PAC1R from the molecular dynamics simulation were compiled through k-mean cluster analysis. The top 10 clusters were used for screening small molecules ZINC library using AutoDock Vina. Top candidates among small molecules and peptidomimetics are subjected to further binding assay test.

31	Joel	Mallory	UCI	Probing the Structural Properties of Small Clusters using the Diffusion Monte Carlo Method	The ground states of small molecular clusters have long been of interest to experimentalists and theorists as their structures are often strongly influenced by the effects of quantum delocalization and zero point motion. The Mandelshtam group is currently implementing a popular method known as diffusion Monte Carlo (DMC) to study the ground state energies, wavefunctions, and structural characteristics of small clusters from water to parahydrogen and their isotopologues. Our initial research focused on assessing the performance of DMC with regard to sources of systematic error or bias (e.g. the random walker population size) for energetically low-lying isomers of the water hexamer using the cheap, empirical TIP4P water potential energy surface (PES). In order to gain a more accurate, qualitative understanding of small water clusters in their ground states from the dimer to the hexamer, we employed the ab intio-based MB-pol PES in conjunction with DMC to determine the isomer fractions of configurations substantially contributing to the wavefunctions. Our work on this front indicates that the ground states of N=2-5 clusters and their deuterated isotopologues are dominated by the global minimum configuration. However, we observe that an isotope shift occurs for the MB-pol water hexamer in which the ground state switches from the global minimum geometry to becoming delocalized over four nearly isoenergetic local minima upon substituting the deuteriums for hydrogens. More recently, our principle aim has been directed toward small parahydrogen clusters and their orthodeuterium isotopologues using the Silvera-Goldman interaction potential. Probing these systems with DMC have proven to be nontrivial due to significant delocalization of the ground state over a vast configuration space that includes numerous basins of attraction and local minima, many of which compete with each other for the ground state. We have performed a rigorous structural analysis of parahydrogen N=19,38 systems and their orthodeuterium N=19,38 isotopologues to ascertain the configurations that contribute appreciable amplitude to the ground state wavefunction. This information is necessary to establish the phase of the ground state, which we determine to be liquid-like or competely liquid for the parahydrogen clusters and solid-like or even amorphous for the more classical
32	Sahil	Gulania	USC	Electronic Structure of Negative Ions (CN- and C_3N-)	In this study, an attempt is made to study the chemistry of negative ions from electronic structure point of view. Due to the presence in interstellar medium (ISM), CN- and C_3N- became first candidates for detailed investigation. Their photodetachment cross-section were computed and compared with the experimental data. Dipole bound states for C_3N- were also looked carefully. The future work will include adding more anions in this list like C_5N-, explaining the process of formation of anions in ISM and detailed investigation for dipole bound states and their characterization.
33	Tirthendu	Sen	USC	Effect of mutations on redox potential of EGFP	Green to red photo conversion, known as oxidative redding, is very common in GFP protein family. GFP protein does not undergo such redding. However, EGFP undergoes redding upon photo excitation. This redding involves an electron transfer pathways. This can be attributed to different protonation state of Chromophore and Glu 222 in GFP and EGFP. We discover Tyr 145 and Phe 165 as probable electron acceptors which are competetive electron acceptors responsible for redding. Several mutations and redox calculations lead to clear understanding of this mechanism. We also try to understand the role of Thr 65 by mutating it with Gly and Ala.This may contribute to enhancing photo stability of FPs.

34	Addis	Fuhr	UCLA	On the Molecular Origin of Intra-gap Emission from CuInSe2-xSx Quantum Dots	CuInSe2-xSx (CISeS) quantum dots (QDs) exhibit several unusual photophysical properties that are distinct from those of structurally similar II-VI QDs. The large Stokes shifts (), for example, inhibits reabsorption losses in luminescent solar concentrators by reducing the spectral overlap between the emission and absorption spectra. On the other hand, the broad linewidths limit their use in high-color-definition displays. A possible explanation for these spectral features is the involvement of intra-gap states containing a localized hole capable of coupling with a conduction band electron for a radiative transition. However, the origin of these intra-gap states, and their role in both emissive and non-emissive decay channels still remain poorly understood. Here, we address these questions with density-functional theory (DFT) calculations. Our results predict the formation of intra-gap states, which arise from either copper anti-site swapping ($CuIn_2-$ + $InCu_2+$), or from excess positive charge accumulated on a lattice copper in order to charge-balance a copper vacancy ($VCu-$ + $CuCu+$, where $CuCu+$ is a Cu^{2+} atom on a Cu^+ site). The theoretical Stokes shifts, predicted by the energy off-set between the localized defect and valence band varies from ~0.3 eV to ~0.7 eV based on the proximity of the Cu-defect with their corresponding charge-balancing paired defect ($InCu^{2+}$ in the case of $CuIn_2-$ and $VCu-$ in the case $CuCu+$). These variations are in excellent agreement with single-dot spectroscopy studies, and suggest that future work on Stokes shift engineering of CISeS QDs should focus on controlling the spatial distribution of Cu-based defects.
35	Saswata	Roy	UCI	Computing photoacidity of molecules through TD-DFT	Photoacids offer an alternative route for light harvesting and storing it as chemical energy. However, structure-property relationship for these photoacids are poorly understood. The source of photoacidity in substituted quinolines and the possibility of the molecules undergoing intersystem crossing is investigated.
36	Bryn	Taylor	UCSD	Investigating Chemokine Receptor CCR2 Dynamics and Druggability by Ensemble Based Approaches	Increased activity of chemokine receptor CCR2 is implicated in inflammatory diseases including two dozen types of cancer, type 1 diabetes, and rheumatoid arthritis. Extensive efforts to develop an effective drug to inhibit CCR2 signaling have been unsuccessful. With the recently resolved structure of CCR2, we perform long timescale molecular dynamics (MD) on the Anton2 supercomputer coupled with a Markov-state model (MSM) framework to address two key challenges: (i) to understand how small molecule antagonists modulate the protein dynamics, and (ii) to develop drugs that bind to novel allosteric sites on the protein. Development and application of this MSM framework will enable widespread use of these approaches to other biological systems.
37	Dibyendu	Mondal	USC	Exploring the Drug resistance of HCV Protease	Nearly 170 million people world wide are affected by Hepatitis C virus (HCV), which causes chronic liver infection. This chronic infection can subsequently lead to cirrhosis of liver and some times liver cancer. HCV, a RNA virus generates different viral proteins like C (core), E1, E2 and non-structural proteins (NS3, NS4, NS5), of which NS3/4A protease has been studied quiet extensively as drug target. Even though several drugs have been developed, their subsequent resistance conferred due to mutation has been a huge hindrance in successfully developing an effective inhibitor. We studied four drugs of NS3/4A protease, which are either FDA approved or under clinical trial, using computational methods to analyze the effect of mutations on their binding. Additionally, we investigated the mechanism of the protease to calculate the vitality values (Kikcat/Km), which can guide us to understand how effective a mutation would be for a virus, which can resist the inhibitor from binding to the protein without affecting its catalytic efficiency. Our EVB calculation showed that the NS3/4A protease follows stepwise mechanism to catalyze the peptide bond cleavage. The calculated kcat from EVB and Km and Ki from binding free energy calculations using PDLD/S-LRA methods show good agreement with the experiments. The molecular details pertaining to resistance are also discussed. We further used this same strategy to predict some mutations for these drugs that have not been studied extensively. Overall, we have tried to show how vitality can be used as a strategy, to predict drug resistance mutation.

#	First	Last	Affiliation	Title	Abstract
38	Raphael	Florentino Ribeiro	UCSD	Continuous Vibronic Symmetries in Jahn-Teller models: local and global properties	This work focuses on the interplay between electronic and vibrational degrees of freedom in a class of strongly-coupled Jahn-Teller systems (JT). In particular, we provide a systematic study of ideal JT models invariant under the action of continuous groups on the electronic and vibrational Hilbert spaces. We emphasize the i) local and global properties of their multi-branched adiabatic potential energy surfaces, (ii) the effects of the Berry phase on the vibronic ground-state symmetry and degeneracy, and (iii) the relevance of our results to more complicated chemical systems without any symmetries. Our study includes models containing strong spin-orbit coupling, as well as those which may be treated as spinless.
39	Benson	Nguyen	CSUF	Hydrogen Peroxide Synthesis Using Defects Sites in Graphene Hydroxide	Hydrogen peroxide (H2O2) is a colorless liquid that is primarily used in industry as an oxidant for wood pulp bleaching and waste water management. Through specific metal catalysis, hydrogen peroxide can be converted into highly reactive hydroxyl radicals that degrade a variety of organic compounds such as greenhouse gases and halocarbons. Industrial hydrogen peroxide is produced though the anthraquinone process via hydrogenation and oxidation of 2-alkyl-anthraquinone. Hydrogen peroxide, itself, is environmentally benign as it decomposes to water and oxygen however, its industrial synthesis is not as environmentally friendly. This process requires dissolved alkyl-anthraquinone mixed with organic solvents followed by liquid extraction to retrieve the hydrogen peroxide. A similar process could function within defect sites of a graphene hydroxide sheet. As a first step towards understanding its suitability for this process, we will compare the catalytic properties of functionalized graphene to the anthrahydroquinone using Density Functional Theory. We will present an analysis of the local minima and transition states and discuss the relative advantages of both systems.
40	Payal	Chatterjee	Western Universiy	Free Energy based design of reversible covalent inhibitors for Calpain2.	Calpains are calcium activated cysteine protease, whose over-activation contributes to many disorders including neurodegeneration. Of the plethora of inhibitors, α-ketoamide based reversible covalent inhibitors are found to be less toxic and more potent. The diketoamide warhead of these peptidomimetic inhibitors directly targets the Sulfur of catalytic cysteine residue via a multistep process, to form a reversible covalent bond. Although some of them have shown considerable selectivity for Calpains over other cysteine protease, the reason for their selectivity might be a contribution of the groups flanking the warhead on one or both sides (P and/or P'). Lately, the two Calpain isoforms in humans viz. calpain1 and calpain2 have been found to play opposite roles in neurodegenerative diseases. Calpain1 have been proven to be neuroprotective, while calpain2 as neurodegenerative, which introduces the need for selective inhibition of calpain2. Achieving selectivity amongst these two isoforms with highly homologous active site is however a challenge. In the present study, we utilize Free Energy Perturbation/Hamiltonian-Replica Exchange Molecular Dynamics (FEP/H-REMD) to understand the contribution of P' groups of α-ketoamide based peptidomimetics inhibitors. This technique utilizes FEP to perturb the primed group and H-REMD to ensure adequate sampling and convergence of the ligand-receptor complex with highly flexible active cleft. The relative binding free energy of α-ketoamide were calculated for both non-covalent and covalent bond states in the two isoforms. Our results suggest that the non-covalent bond state can capture majority of the selectivity, although extra caution is needed for setting up each protein model.
41	Carlos	Jimenez Hoyos	Caltech	TBA	TBA

#	First	Last	Affiliation	Title	Abstract
42	Christine	Pham	Western Universiy	Computational Investigation of Piezo1 Channel Agonist Binding Site	Piezo proteins are mechanosensitive cation channels that play essential roles in diverse mechanotransduction processes resulting in touch sensation, proprioception, blood pressure regulation, and proper vascular developments (1-6). Gain-of-function mutations in both isoforms have resulted in rare diseases (7-9). The aim of this study is to use computational programs to identify potential binding site of a selective agonist Yoda1 on Piezo1, and how Yoda1 activates Piezo1 (10). A wild-type Piezo1 and Yoda1-insensitive Piezo1 mutant models were built based on Cryo-EM structure of mouse Piezo1 from the Protein Data Bank (PDB ID 3jac). The models were imbedded in homogenous lipid bilayer membranes and solvated in water and 0.15M of NaCl using CHARMM36 force field through CHARMM-GUI web site. All atom molecular dynamic simulations were performed using AMBER 16. Root mean square deviation cluster analyses were performed to extract distinct protein conformations from the trajectories and docking was done using Autodock4.2. We observed several Piezo1-specific binding sites for Yoda1. Different binding poses and protein-agonist interactions wild-type and mutant Piezo1 will be further analyzed to gain insights in the mechanism of activation of Piezo1 channel. These finding will be used to design potential antagonists.
43	Shane	Anderson	Western Universiy	Structural Activation pathway of the AT1R determined via computationally derived models	It is accepted that GPCRs structurally rearrange, leading to GDP disassociation and GTP association with the Gα subunit; however, the dynamic mechanism underlying how GPCRs activate G proteins remains unknown. A recent examination of 27 crystalized inactive and active state GPCRs revealed convergence of residue rearrangement near the GPCR-Gα subunit interface. To examine dynamic changes involved in activation of the Angiotensin (Ang) II type 1 receptor (AT1R), we utilized molecular dynamic (MD) simulations of an empty-AT1R, constitutively active (CA) AT1R, and Ang II-bound to both the wild-type and CA receptors. After measuring RMSD of the helical residues and Ang II, as well as intra-contact residues, salt bridges, hydrogen bonds, and helical rotations, it was determined that the CA and Ang II-bound AT1R structures were stable yet inactive and Ang II resided in a low-affinity state. A C-terminal fragment of Gαq, similar to that used to crystallize active-state Rhodopsin (PDB: 3PQR), was aligned and inserted into the bottom of one Ang II-AT1R complex and an additional 300 ns MD simulation. Analysis of the inserted Ang II-AT1R- Gαq complex revealed a stable active state structure, whereas the aligned structure remained inactive. Moreover, Ang II appeared to lock into place with insignificant variation, representing a high-affinity state, mirroring pharmacological data and reinforcing the requirement of Gα to reveal the active structure. Lastly, the Gα fragment should be arranged logically into the void at the bottom of the receptor to gain an active GPCR.
44	Luke Nambi	Mohanam	UCI	Perturbative Approach to Ultrafast Intersystem Crossing in Nonadiabatic Molecular Dynamics	While intersystem crossing (ISC) between singlet and triplet states is slow in most molecules containing first- and second-row atoms, some systems, such as benzophenone, exhibit ultrafast ISC, which affects excited-state dynamics and photochemical reactions. In transition metal compounds such as tris-(bipyridine)ruthenium2+, ultrafast ISC is common and competes with spin-conserving deactivation pathways. Nonadiabatic molecular dynamics (NAMD) is the method of choice to investigate and predict the effect of ultrafast ISC computationally. We present a perturbative scheme for including this ISC through spin-orbit coupling in NAMD simulations within the time-dependent density functional theory (TDDFT) framework.The spin-orbit coupling is obtained from the trace of the one- and two-electron Breit-Pauli spin-orbit coupling operator with the transition density matrix. Preliminary results for several molecules and density functionals are presented. We report applications to validate our approach, and discuss its scope and limitations.
45	Matthew	Welborn	Caltech		
46	Philip	Shushkov	Caltech		
47	Jorge	Rosa	Caltech	Path-Accelerated Molecular Dynamics	An approach that exploits the path-integral representation of the marginal distribution for the time-evolution of a classical system to integrate MD trajectories is developed and applied to simple models obeying Brownian dynamics. Using parallel algorithms to evaluate the path integrals, we demonstrate the time-parallelization capabilities of the method by achieving hundred-fold speedups over the conventional Euler integration scheme.

48	Feizhi	Ding	Caltech	Embedded Mean-Field Theory for High-Efficiency Electronic Structure	Processes involving electronically excited states are crucial for many functions of biological systems and devices. Examples include the photo-excitation and charge transfer in natural and artificial photosynthetic centers. Understanding such processes would require a reliable quantum chemical description of excited states, at a computation cost that is feasible for large length-scale and long-time-scale simulations. While highly accurate wavefunction methods (such as the equation-of-motion coupled cluster) are only applicable to very small systems, time-dependent density functional theory (TDDFT) offers a good compromise between cost and accuracy, and has been routinely applied to rather large systems with up to several hundreds of atoms. However, reliable treatment of excited states in even larger and more complex systems (such as the photosynthetic reaction center) remains a significant challenge in theoretical chemistry. In response to this situation, we have developed a time-dependent embedded mean-field theory (TD-EMFT) for the seamless, multi-level description of the excited state electronic structure of complex molecular systems and materials. In this approach, the full system is partitioned into two subsystems. The subsystem in which the excitation processes occur is treated with a high-level method such as hybrid-DFT, and the surrounding environment is described using a lower and cheaper method such as density functional tight binding. The electronic response of the environment to the excitation is included via the so-called interaction kernel. We show through a number of tests that this method performs accurately and thus provides a promising tool for treating excited states in large systems.
49	Jae	Yeon	Western Universiy	A nonlinear regression approach to optimizing binding affinities for ARB-AT1R complexes via autodock4 for the understanding of ARB resistance	Angiotensin II type 1 Receptor (AT1R) blockers (ARBs) are commonly prescribed drugs for patients with high blood pressure, heart failure, and chronic kidney disease. However, ARBs are not always as effective as predicted and there are patients that are considered ARB resistant. There are 103 non-synonymous polymorphisms within the first and last amino acid of the crystal structures of the AT1R that may alter binding affinity. To generate a stable empty AT1R, PDB:4zud minus olmesartan was modeled utilizing Amber16 for 150 ns in an 87% POPC and 13% cholesterol membrane. Each aforementioned polymorphism was created via MOE and minimized prior to docking via autodock4. A modified Levenberg-Marquardt non-linear regression method was used with autodock4 to ensure wild type AT1R-ARB affinities matched published experimental affinities. By manipulating the Z-axis and gridbox spacing (Å) for each ARB, binding affinities were derived and matched to previous experimentally derived affinities. The gridbox parameters for each ARB were then used for each polymorphic AT1R model for the determination of affinity for each ARB-AT1R combination. In Total, 93,600 drug-receptor complexes were analyzed with the data indicating polymorphisms fall into two general categories: ARB specific resistance and total ARB resistance. Polymorphic AT1Rs displaying ARB specific resistance have wild-type affinities for a subset of ARBs; whereas, total ARB resistance, such as W84C, indicates that all ARBs are ineffective. This research is beneficial as it brings personalized medicine to ARB therapy specifically by identifying the ARB that would coincide with the patient's AT1R sequence.
50	Wesley	Botello-Smith	Western Universiy	Computational Investigation of Phosphorylatio n Induced Serine / Threonine Kinase Activation and Modulation of Allosteric Regulation due to Point Mutation	Serine / Threonine kinase receptors (STKR) play important roles in a number of regulatory cellular signaling pathways. Elucidation of the dynamic structural changes that occur during their transition from inactive to active state is of great interest to the computational biology community. Furthermore, several point mutations of the type I receptors, near the binding site for a large inhibitory peptide, are known to induce 'leaky' signaling. A better understanding of the mechanism by which these point mutations disrupt this inhibitor's allosteric signaling is also of strong importance. Structural comparison between simulations of the type I STKR wild type with and without this inhibitor bound revealed a key R-D salt bridge located near the ATP binding site. This salt bridge, apparently, plays a strong role in regulatory inhibition of ATP binding. Here, we present a wavelet guide principal component analysis (WAFEX-PCA) used to capture the relevant motions leading to activation induced by phosphorylation of Type 1 STKR, particularly, as related to the necessary dissociation of the regulatory R-D salt bridge. Finally, analysis of atomic motion correlation networks revealed how a point mutation near the allosteric binding site, experimentally known to cause 'leaky' signaling, induces a perturbation of the associated allosteric interaction network connecting the binding protein domain to the inhibitory R-D salt bridge.

51	Shane	Parker	UCI	Nonlinear optical properties from TDDFT: Trials and tribulations	Nonlinear response theory plays a central role in theoretical materials chemistry and applications of nonlinear response theory within time-dependent density functional theory (TDDFT) are increasingly important, from the calculation of nonlinear optical properties used to characterize complex materials to the excited-state properties and couplings needed to simulate non-adiabatic molecular dynamics. I will present an efficient implementation of the TDDFT quadratic response function, including the computation of excited state absorption spectra of perylene diimide dimers, two-photon absorption spectra of twisted conjugated porphyrins, and hyperpolarizability of octupolar calixarenes. Distressingly, recent descriptions of unphysical divergences in excited-state properties and the inconsistent behaviors of multiphoton processes near single-photon absorption resonances have called into question the general applicability of existing nonlinear response theories. Finally, using the aforementioned systems as examples, I will sketch the successes and failures of existing nonlinear response methods and discuss possible routes for resolving the deficiencies in nonlinear response theories.
52	Jim	Mcsally	UCI	Computational Studies of the Hoogsteen Base-pair in RNA and DNA.	The true biological function of the Hoogsteen (HG) base pair is still under investigation. The HG base pair is a conformational state in nucleic acids that is a 180o rotation of the glycosidic bond of the purine nucleotide from traditional Watson Crick (WC) pairs. This allows a different set of hydrogen bonds to form with the pyrimidine counterpart, and changes the physical properties observed from the major and minor grooves in double stranded nucleic acids. There have been many studies investigating the HG base pair in DNA, but little is known about the ability of the HG base pair to form in RNA. Here work, using Biased Molecular Dynamics and Equilibrium Molecular Dynamics, will show the relative instability of the Hoogsteen base pair in various nucleic acid contexts. Understanding the physical limitations of each nucleic acid's ability to form the HG base pair, may lead to clarification on the biological role of the HG base pair.
53	Sree Ganesh	Balasubr amani	UCI	Non-covalent interactions using orbital-optimized random phase approximation	The correlation energy within the random phase approximation (RPA) is an inreasingly popular method for computing electronic ground-state correlation energies. RPA does not require empirical input, is relatively accurate for a large range of covalent and noncovalent interactions, and only slightly more computationally expensive that second-order Møller-Plesset perturbation theory. Nevertheless, the conventional 'post Kohn-Sham' approach, which evaluates the RPA correlation energy using Kohn-Sham orbitals obtained with a semi-local exchange-correlation potential, underbinds a variety of van der Waals (vdW) complexes, even though RPA captures the correct physics to describe dispersion interactions at all ranges. We present a new approach based on optimized RPA orbitals that improves the description of noncovalent interactions and reduces the dependence on the KS reference determinant. In addition, orbital optimized RPA is found to yield qualitatively correct potential energy curves for beryllium dimer as well as other systems with strong static correlation. Another promising application of orbital optimized RPA are open-shell systems, as shown by comparison to benchmark data for a set of small open-shell species.
54	Charles	Zhang	Western Universiy	Achieving Proper Docking Parameters for Zinc Incorporated in Metalloenzyme s to Model Drug Binding	Antibiotic resistance through the production of β-lactamases is an urgent and complex issue. β-lactamases have the ability to hydrolyze commonly used β-lactam antibiotics, such as penicillins, cephalosporins, carbapenems, and monobactams. Most β-lactamases inactivate β-lactams through the use of an active site serine. Class B β-lactamases incorporate zinc ions in their active site and are deemed metallo-β-lactamases (MBLs). Clinically relevant MBLs belong to the New Delhi MBL (NDM), Verona Integron-borne MBL (VIM), and Imipenemase (IMP) families. There are currently no clinically available MBL inhibitors. Molecular modeling through the use of docking is generally used as a first step to study binding interactions between β-lactamases and different antibiotics/potential inhibitors. Issues arise for MBLs where binding affinities and bond lengths from docking commonly deviate from what is found in crystal structures. This is largely due to the improper atom parameters and charges from the base docking programs, mainly in reference to the zinc ions. Many publications use these base parameters and are therefore receiving inaccurate binding data. Our study determined proper zinc ion parameters and parameters to achieve docking results that are consistent with crystal structures of NDM-1, VIM-2, and IMP-1 enzymes in complex with inhibitors through the use of AutoDock 4.2. Using these adjustments, the enzymes were subsequently docked with clinically used antibiotics and binding affinities were compared to the experimental catalytic efficiencies determined in steady-state kinetic experiments in our lab.

55	Emilia	Pecora De Barros	UCSD	Investigating the dynamics of designed ligand-binding proteins	Protein design constitutes a challenging but promising area in biochemistry. Custom-designed ligand-binding proteins, in particular, present promising applications in small-molecule sensing, diagnostics, and in therapeutic scavenging of toxic compounds. Some of the challenges in designing ligand-binding protein lies in the creation of a binding site that results in high affinity interaction but is also pre-organized and does not collapse in the absence of ligand. Here, we use molecular dynamics simulations to assess the cavity stability of designed proteins that have been tested experimentally. Our apo simulations provide information on the cavity pre-organization, while holo simulations indicate protein-ligand affinity and correlate well with experimental observations. The results obtained can be used to guide further steps in protein design, and will be combined to select appropriate metrics for the prediction of binding affinity of future un-tested proteins, aiding the protein design methodology.
56	Jeongmin	Kim	Caltech	Toward Understanding the Solid Electrolyte Interphase: Ion Transport and Electron Transfer at the Electrode-Electrolyte Battery Interface	Understanding and optimizing interfacial properties of batteries are crucial for increasing battery safety and longevity [1]. However, fundamental understanding is still elusive. At the interface between electrode and electrolyte a solid electrolyte interphase (SEI) layer forms immediately and spontaneously. The SEI should be ionically conducting but electronically insulating to protect against further uncontrollable and unwanted reduction of the electrolyte that would lead to catastrophic failure of batteries. In this poster, we present simulation results of reduction and transport of Li+ cation in the SEI region between model metal electrodes. We use the canonical solid electrolyte, poly (ethylene oxide) (PEO), as a model for the SEI and polarizable metal electrodes are employed via the constant potential method [2]. The charge distribution on the electrode may reflect conformational changes at the interface, which would, thereby, change electrochemical properties at the interface. That is because PEO chains chelate Li+ cations to dissolve them, spending a dihedral penalty. Moreover, we compare the results in PEO to those in diglyme electrolyte that is chemically equivalent to PEO but a short oligomer to elicit fundamental differences in the SEI from conventional liquid electrolyte. [1] K. Xu, Chem. Rev. 114, 11503 (2014) [2] S. K. Reed at al., J. Chem. Phys. 126, 084704 (2007); Z. Wang et al., J. Chem. Phys. 141, 184102 (2014)
57	Guo	Chen	UCI	Complexes of rare-earth and actinide elements in unconventional oxidation states	The +2 oxidation state has recently been identified in trigonal silylcyclopentadienyl complexes of Y, lanthanides (except radioactive Pm), as well as Th and U. Density functional theory (DFT) calculations suggest that the trigonal coordination environment stabilizes a $dz2$ orbital that facilitates the formation of the new +2 ions ($Y2+$, $La2+$, $Ce2+$, $Pr2+$, $Gd2+$, $Tb2+$, $Ho2+$, $Er2+$, $Lu2+$, $Th2+$, and $U2+$). Here, we show that the success in obtaining metal complexes with low oxidation states can be generalized to both lighter and heavier part of the periodic table. DFT and time-dependent DFT (TDDFT) calculations have helped to identify the first crystallographically characterizable $Sc2+$ complex, {Sc[N(SiMe3)2]3}−,[1] and the first $Pu2+$ complex, {Pu[C5H3(SiMe3)2]3}−.[2] Unlike $Th2+$ and $U2+$, the $Pu2+$ ion has predominantly a 5f6 electron configuration with some 5f56d1 mixing, reflecting the change in relative energy of 5f and 6d orbitals across the actinide series. The newly discovered complexes have the characteristic strong absorption in the visible region and exhibits unusual reactivity, e.g. small molecule activation. [1] D. H. Woen, G. P. Chen, J. W. Ziller, T. J. Boyle, F. Furche, W. J. Evans. Angew. Chem. 2017, 129, 2082−2085. [2] C. J. Windorff, G. P. Chen, J. N. Cross, W. J. Evans, F. Furche, A. J. Gaunt, M. T. Janicke, S. A. Kozimor, B. L. Scott. J. Am. Chem. Soc. 2017, 139(11), 3970−3973.

58	Anupam	Chatterjee	UCI	Elastic properties of contractile tails in pre- and postcontraction states: Insight from equilibrium MD simulations	Contractile tails are found in a wide range of biological nanomachines involved in cell puncturing mechanisms. Two such related `contractile systems' are the bacteriophage T4 and R-type pyocins. During a fascinating injection process, the tail sheaths of both systems contract from the so-called ``extended state" to around half of their length accompanied by the release of stored elastic energy in the sheath. Despite the great population and importance of contractile systems, many fundamental details of their injection machinery and dynamics are still unknown. In this work, we calculate the twisting and bending stiffness coefficients of a helical tail sheath strand of bacteriophage T4 and r-2 pyocin, in both extended and contracted states, using massively parallel MD simulations of about one fifth of the entire sheath structure. These coefficients are then used in a dynamic continuum model to simulate the entire injection process of both systems. The calculated coefficients correctly predict that the sheath strand has greater flexibility in the extended state for both systems. The dynamic model for phage T4, described in a separate work, predicts an energy of contraction which is very close to the reported experimental free energy of contraction.
59	Pushp	Bajaj	UCSD	Toward a quantitative molecular level understanding of ion-hydration using many-body potential energy functions	Despite continuous effort, a unified understanding of how specific ions affect the structure and dynamics of water remains elusive. In this work, we present many-body potential energy functions, called MB-nrg, for halide ions (F-, Cl-, Br-, I-) in water, derived entirely from CCSD(T)-F12 data in the complete basis set limit. The potentials build upon our highly-accurate "first principles" water potential, MB-pol, which is used here to describe the water-water interactions. MB-nrg potentials include many-body effects for all system sizes by taking into account explicitly the two-body and three-body interactions, and all higher order interactions implicitly through a mean field approximation. Extensive comparisons of interaction energies and vibrational frequencies are presented with calculations from several DFT models and polarizable potentials (such as i-TTM, and AMOEBA), and experimental measurements, which exhibit the unprecedented accuracy of the MB-nrg potentials.
60	Sandra	Brown	UCSD	Monitoring Water Clusters "Melt" Through Vibrational Spectroscopy	The ability of small water clusters to serve as model systems for elucidating the complicated structure and dynamics of bulk, condensed-phase water has made them the subject of intense and on-going interest. Playing a special role as the prototypical system for studying hydrogen-bonding in water is the water hexamer, as it is the smallest water cluster whose minimum energy configurations exhibit three-dimensional structures similar to those found in bulk water. In this work, we monitor the "melting" of the water hexamer from well-defined "solid-like" structures to disordered "liquid-like" structures by tracking the evolution of both the vibrational spectrum and the distribution of orientational bond order parameter as a function of temperature. To achieve this, we combine the unrivaled accuracy of the MB-pol potential energy surface with quantum dynamics methods which are able to capture both the anharmonicity and quantum effects that are critical for an accurate description of hydrogen-bonded systems. A range of temperatures over which molecular-level "melting" occurs is identified for both $(H2O)6$ and $(D2O)6$, with the greater quantum-character of the $(H2O)6$ cluster resulting in a lower melting-temperature range. Experimentally, the temperature-controlled determination of vibrational spectra for neutral water clusters remains out of reach. Thus, while we find that our results agree with the limited, low-temperature experimental data which is presently available, this work can be seen as a testament to the predictive capabilities of theory.
61	Vamsee	Voora	UCI	Orbital Optimised Random Phase Approximaion	
62	Daniel	Jacobson	Caltech	TBA	TBA
63	Ethan	Phan	USC	Solvent Thermodynamics Driving Force Controls Stacking Interactions Between Polyaromatics	Monte Carlo simulations are used to probe the effects of solvent in determining stacking conformations of different polyaromatic hydrocarbons

64	Ty	Roach	San Diego state	Entropy in the Tangled Nature Model of Evolution	Applications of entropy principles to evolution and ecology are of tantamount importance given the central role spatiotemporal structuring plays in both evolution and ecological succession. We obtain here a qualitative interpretation of the role of entropy in evolving ecological systems. Our interpretation is supported by mathematical arguments using simulation data generated by the Tangled Nature Model (TNM), a stochastic model of evolving ecologies. We define two types of configurational entropy and study their empirical time dependence obtained from the data. Both entropy measures increase logarithmically with time, while the entropy per individual decreases in time, in parallel with the growth of emergent structures visible from other aspects of the simulation. We discuss the biological relevance of these entropies to describe niche space and functional space of ecosystems, as well as their use in characterizing the number of taxonomic configurations compatible with different niche partitioning and functionality. The TNM serves as an illustrative example of how to calculate and interpret these entropies, which are, however, also relevant to real ecosystems, where they can be used to calculate the number of functional and taxonomic configurations that an ecosystem can realize.
65	Zhedong	Zhang	UCI	Relaxation of polariton and cooperativity in microcavities monitored by third-order resonant spectroscopy	
66	Prasoon	Saurabh	UCI	Two-dimensional infrared spectroscopy of vibrational polaritons of molecules in an optical cavity	
67	Saleh	Riahi	UCI	Proton Permeation in the Hv1 Proton Channel	
68	Kaushik	Nanda	USC	Non-linear optical properties of closed- and open-shell species with EOM-CCSD	Design of novel organic materials with enhanced/tunable nonlinear response impacts many applications in chemical, biological, and materials sciences. Traditionally, design of nonlin- ear materials has focused on closed-shell motifs. Open-shell systems are gaining attention as candidates with enhanced nonlinear response. However, the role of electronic structure of open-shell species in their nonlinear response is unclear. We will present robust methods for calculating two-photon absorption spectra and nonlinear properties such as excited-state dipole polarizabilities within the equation-of-motion coupled- cluster singles and doubles (EOM- CCSD) framework, which can accurately describe the electronic structure of a variety of closed- and open-shell systems. Results for prototypical closed- and open-shell organic molecules will be presented. We will also present theoretical tools that help in interpreting these results and establishing structure-property relationships for these nonlinear properties.

69	Brooke	Zhou	Caltech	Fock-Corrected DFT: parameterization and application in complex systems	Quantum chemistry calculations of large systems have been challenging for traditional DFT methods with complex functional and large basis set in terms of calculation costs. We have been developing Fock-corrected density-functional theory (FCDFT), a semi-empirical method that can in principle achieve comparable accuracy to any current DFT methods with the cost of only minimal basis simple functional DFT calculations. FCDFT has a DFTB-like Fock-matrix correction term by Slater-Koster transformations and a pairwise potential term that depends on interatomic distances. It also contains the full Kohn-Sham treatment of Coulombic electrostatics. With similar calculation cost, FCDFT performs better than either minimal-basis DFT or DFTB in terms of correcting basis-set incompleteness and properly accounting for electrostatics. Choosing LDA/STO-3G as the method to be trained, we have calculated both diagonal-only and full-matrix Fock-correction parameters by Broyden–Fletcher–Goldfarb–Shanno (BFGS) minimization of square-root loss-function. We also demonstrated that FCDFT is a perfect choice for the low level method in embedded mean-field theory (EMFT) calculations. EMFT calculation with FCDFT as low-level method in zeolite catalyst for alkane cracking, decanoic acid and ester has achieved satisfying accuracy compared to high-level results but with much lower calculation cost. The next steps will be to extend the current training set to include more elements, to try different Fock-correction formulae and to implement new parameterizations strategies.
70	James	Fields	UCI	An Arginine-rich Cytosolic Loop is Critical For the Modulation of the Water Permeability of Aquaporin 0	Aquaporin 0 (AQP0), the major intrinsic protein of the eye lens, plays a vital role in maintaining lens clarity by facilitating water transport. AQP0 reduces its osmotic water permeability constant (Pf) in response to increases in the external calcium concentration, an effect that is mediated through an interaction with calmodulin (CaM). Phosphorylation reduces calcium sensitivity of AQP0 Pf , either locking the pores either low or high. Despite recent structural characterization of the AQP0-CaM complex, the mechanism used by CaM to modulate AQP0 remains poorly understood. We employed a combination of Brownian and molecular dynamics simulations to identify the critical features of the AQP0-CaM interaction. Brownian dynamics (BD) simulations suggest that serine phosphorylation of AQP0 does not significantly reduce CaM-binding to the whole AQP0 protein, in contrast to the experimental observation that phosphorylation does significantly reduce binding to C-terminus AQP0 peptides. Comparative MD simulation studies show that AQP0 phosphorylation changes contacts between AQP0 and CaM, particularly at a small arginine-rich loop on the AQP0 cytosolic face. This charged loop allosterically couples CaM to the second constriction site residues of AQP0 through an interaction with R156. Additionally, we observe that R153 increases the size of the pore opening through an interaction with the Y149 hydroxyl group, which is necessary for maintaining high permeability states of AQP0. Experimental and simulation data support the notion that serine phosphorylation of AQP0 changes the calcium sensitivity
71	Andrew	Geragotelis	UCI	Multi-Microsecond Molecular Dynamics Simulations of the Hv1 Proton Channel	The voltage-gated proton channel, Hv1, is a membrane protein that plays roles in a variety of cellular processes including proton extrusion, pH regulation, and the production of reactive oxygen species. In order to characterize the structure and transition between the closed and open states of Hv1 in a realistic membrane environment, we used multi-microsecond molecular dynamics (MD) simulations. Specifically, we carried out MD simulations of the mouse chimera trimer and monomer in a fully hydrated POPC bilayer, as well as human Hv1 (hHv1; starting from a homology model built from mHv1cc). We found that all three of the constructs considered (mHv1cc trimer, mHv1cc monomer, and hHv1 monomer) were stable at zero potential on the timescale of several microseconds. Additionally, the monomer hHv1 model was subjected to hyperpolarizing and depolarizing transmembrane potentials. The structure underwent only minor changes under hyperpolarizing potential. However, under a depolarizing potential, we observed a large conformational change of the protein through the outward movement of the S4 helix by approximately 8 Å. This transition led to a rearrangement of the internal salt-bridge network and allowed more waters into the pore as well as an increased stability in the hydrogen bond pathways, suggesting that it is an open state. We validated our atomistic hHv1 models with a variety of experimental data, including gating charge measurements and binding of the known inhibitor, 2-GBI, at the intracellular side of the selectivity filter, as well as a cadmium ion bridging assay.

72	Gerardo	Mendoza	San Diego State U	Effect of the π-π interactions on the Glass Transition Temperature of Nanometer Thin Polystyrene Films	The glass transition in free-standing films of linear and cyclic polystyrene (PS) was studied to better understand the experimentally found relationship between the glass transition temperature (Tg) and film thickness. United-atom molecular-dynamic simulations were performed on free- standing films of varying thicknesses. Data confirmed the positive correlation between Tg and film thickness, i.e. Tg decreases as film thickness decreases. At 20 nm the difference is less than 1%, while at 2.5 nm the difference is 13% for linear and 9% for cyclic chains. Recent studies show that a larger number of end groups inhabit the interfacial layer rather than the middle of the film and that a deficit of phenyl groups exists in the interfacial film layers nearly 1 nm below the surface. The large number of end groups would increase interfacial layer mobility while the deficit of phenyl groups would weaken the phenyl-phenyl aromatic (π- π) interaction which would lead to a lower Tg in thin films. The cyclic polystyrene chains lack end groups but have an observed deficit of phenyl rings comparable to that in linear polymers. Therefore, the chain ends alone cannot be the only cause for the observed Tg dependence on the thickness of thin PS films. It appears that the π-π interaction seems to be an important cause as well.
73	Krista	Parry	UCI	Method for direct comparison of MD simulation to experimental XPS data	
74	Vy	Duong	UCI	Oxetane-based Polyketide Surrogates to Probe PKS Enzyme-Substrate Complexes	Polyketide natural products are a large and diverse class of secondary metabolites of high impact to human health. Type II polyketides are biosynthesized by a type II polyketide synthase (PKS) characterized by 5-10 stand-alone enzymes that form complexes in solution. PKSs have been heavily studied due to their ability to efficiently biosynthesize complex small molecules and their potential to be engineered for combinatorial biosynthesis. To interrogate PKS-substrate complexes more broadly, we sought to generate probe molecules that more closely mimicked the natural substrates. The oxetane ring has achieved exalted status in medicinal chemistry over the past decade, owing primarily to the efforts of Carreira, Müller, and co-workers. The carbonyl–oxetane replacement strategy has never been used to study questions in polyketide biosynthesis. Here we present the synthesis of an oxetane-based PKS substrate analogue 1 and demonstrate its applicability by co-crystallizing it with the enzyme DpsC from the daunorubicin type II PKS from Streptomyces peucetius. Our co-crystal structure, in combination with molecular dynamics (MD) simulation data, allowed us to glean mechanistic insights for the ketosynthase (KS) activity of this novel, dual-functioning enzyme.
75	Eleftherios	Lambros	UCI	Structural Characterization of Copper-p53	Copper and metal based coordinate compounds are beginning to integrate their way as potential anti-cancer drugs. The copper in such compounds have been shown to interact with p53 and replace the native zinc. Despite this, no structural characterization of copper bound p53 has been produced. Here, we use computational modeling to create a structural characterization of copper bound p53. The charge of the copper in the zinc site, along with the protonation of the surrounding cysteine ligands was determined via QM examination, and the corresponding force constants for bonds, angles and dihedrals were calculated. We show that copper may in fact stabilize certain loops of p53 leading to p53, despite having less rigid binding character.