ARIZONA STATE UNIVERSITY

Department of Physics

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ASU Department of Physics
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Abstracts

(Alphabetical by Presenter's First Name)
(#) Indicates Poster Number
* Indicates Students Eligible for Tsong Prize

Aurora Ireland (1)*

Title: A Determination of the Partial Decay Width for the hb -> etab gamma Radiative Transition of Bottomonium
Faculty Mentor: Dr. Martha McCartney
Abstract: Theoretical values for the currently unmeasured partial decay width for the bottomonium electromagnetic decay channel hb(1P) -> etab(1S) gamma were established through two methods. The first approach relied on the presumption of a constituent quark model interacting via a simple static potential while the second stemmed from a coupling constant term in the effective Lagrangian. Both approaches yielded values which were found to agree exceptionally well with the predicted range for this partial width.

Brandon Thornton (3)*

Title: Electrodynamic Simulations -- Terminating the Finite-Difference Time-Domain Lattice
Faculty Mentor: Dr. Maxim Sukharev
Collaborators: Andre Brewer M., Clark Miller, James Degraffenreid
Abstract: The focus of this research is constructing and validating an absorbing boundary condition that terminates a Finite-Difference Time-Domain lattice. This lattice is a computing structure which is used to simulate the propagation of electromagnetic radiation and its interaction with materials by replacing the derivatives of Maxwell's equations with finite-difference operations. The absorbing boundary condition employed here is the Convolutional Perfectly-Matched Layer (CPML), a refined version of the PML proposed by Berenger. Oneadvantage that the CPML confers compared to other absorbing layers is its ability to be overlayed onto dispersive material with minimal restructuring of its update equations. Presented here are a brief overview of the finite-difference algorithm, the mathematics of the CPML, and the simulations used to test the CPML.

Claire Landstrom (4)*

Title: TEM Image Processing
Faculty Mentor: Dr. Christian Dwyer
Abstract: TEM images tend to be imperfect replications of the original specimen due to alterations of the electron beam by the effects of magnetic lenses, as well as detection of the beam in image formation which introduces noise to the final image. Using the program Matlab, a mathematical work space and filtering functions can be created to either counteract the lens action on the beam wave or used to reduce unwanted spatial frequencies in the image. Both corrections make use of Fourier transforms, momentum space, and low-pass filters.

Curtis Peterson (5)

Title: Periodic Advection-Diffusion-Reaction Systems
Faculty Mentor: Dr. Wenbo Tang
Abstract: Many physical systems, such as the Belousov-Zhabtinsky reaction or a phytoplankton bloom, experience oscillatory behavior in their concentrations of a time-changing flow topology. Such systems can be modeled by a modification to the advection-diffusion-reaction (ADR) equation that describes the scalar concentrations over time across a spatial domain of chosen dimensionality. An inhomogeneity is added to the ADR equation whose long-term behavior is that of a limit cycle. This results in a change in the behavior about hyperbolic regions, such that abnormally long homogenization times are observed as opposed to the logistic case where they are characterized by short homogenization intervals.

Ian Kenney (6)*

Title: Calculation of small-molecule transfer free energies in various solvents
Faculty Mentor: Dr. Oliver Beckstein
Collaborators: Bogdan I Iorga
Abstract: The free energy to transfer a small molecule from water into another solvent such as octanol or cyclohexane is an important quantity in predicting how small, drug-like molecules distribute throughout the body. We developed a computational protocol to predict transfer free energies with atomistic molecular dynamics (MD) simulations. Our MDPOW package is an automated pipeline that sets up and orchestrates all the simulations required for a transfer free energy calculation. The method is based on alchemical solvation free energy calculations ("free energy perturbation", FEP) in the individual solvents (water, octanol, cyclohexane are currently implemented). In order to optimize the simulation protocol, we examined the effects of changing different simulation parameters on solvation free energies, including assessment of finite size effect, thermodynamic ensemble (NVT vs NPT), and choice of the computational thermostat. Our current "best-practice" protocol consists of NPT simulations using a stochastic integrator and Parrinello-Rahman pressure coupling, separate decoupling of Coulomb and Lennard-Jones interactions (with soft cores), and 20 ns simulation per FEP window for a total of 470 ns MD simulation per hydration free energy calculation. We found no difference between using the thermodynamic integration (TI) versus Bennett-acceptance ratio (BAR) method to calculate the free energies from the MD data. MDPOW was tested on 92 small molecules with known solvation free energies and partition coefficients. The overall average unsigned error was 0.95 for the water-octanol partition coefficient and 0.94 for water-cyclohexane. Detailed analysis suggests that the largest source of error remains the hydration free energy calculation. MDPOW is implemented using Python and Gromacs and is available under the GNU Public License from https://github.com/Becksteinlab/MDPOW.

Jacory Parker (7)*

Title: Temperature-dependence of Transport Properties of Tunnel Junction
Faculty Mentor: Dr. Tingyong Chen
Collaborators: Sarah Galvin, Ji Zhang, Bochao Li, Gejian Zhao, T. Y. Chen
Abstract: In a magnetic tunnel junction (MTJ), two ferromagnetic metals are separated by a thin dielectric barrier with a thickness from a few angstroms to a few nanometers. The tunneling probability depends on the magnetic orientations of the two metals. This can be utilized to sense very small magnetic field of nT and is being used as read head in current magnetic hard drives. It has been proposed that improved sensitivity to pT can enable MTJ to detect signals from human brain.
However, the sensitivity depends crucially on the quality of the dielectric layer, which is often inferred from the transport characteristics R(V) of the junction. Previously, a Simmons formula with approximation at zero temperature for a square potential is often used to extract the barrier properties only in intermediate voltage. Here we present a numerical realization of the Simmons model without approximation and show that R(V) depends strongly on temperature. Now the barrier properties of a tunnel junction can be extracted at any temperature, for any potential, and at any voltage range.

Jonathon Barkl (8)*

Title: Photochemistry with Diamond
Faculty Mentor: Dr. Anna Zaniewski and Dr. Robert Nemanich
Abstract: In this project, we are exploring thin films of diamond on various substrates for photochemistry through electron emission induced by light in the visible spectrum. Diamond is unique as a semiconductor due to its large 5.5 eV band gap, and can have a negative electron affinity, meaning the conduction band edge is at a higher energy than the vacuum. This property allows the electrons emitted through photoemission to be used as an energy “reservoir” for energy intensive reduction reactions, such as the reduction of nitrogen gas to ammonia. This project will explore the properties of the diamond films, substrates, and experimental setups in order to determine if photoemission and chemistry are possible with diamond in the visible light spectrum, with lower photon energies than previously demonstrated. This will require the lowering of the effective work function, the energy required to excite electrons from the valence band to the conduction band. The first phase of this project will be to recreate previous experimental results achieved using ultraviolet light on diamond films on molybdenum substrates. In the second phase, we will study the physical properties of the diamond films, various substrates, and other properties in order to achieve the necessary low effective work function.

Kathleen Clark (9)*

Title: Survey of Ion Coordination Geometries of Structures in the Protein Data Bank
Faculty Mentor: Dr. Oliver Beckstein
Collaborators: David Dotson
Abstract: According to some estimates, between 30% and 40% of all proteins depend on interactions with ions to perform their function. Ions can be a part of an active site in an enzyme, part of a substrate, or play a structural role. In order to understand the molecular mechanisms in all of these cases, it is important to have an accurate description of the interactions of these ions with amino acid sidechains, the protein backbone, water molecules, and cofactors. An automated analysis method was developed to analyze cations contained in crystal structures in the RCSB Protein Data Bank (PDB). The ion coordination geometries of the most prevalent monovalent cations in the PDB (sodium, potassium, lithium, and thallium) were analyzed from the radial distribution functions of oxygen atoms around ions. Monovalent cations coordinate oxygen atoms within about a 6 Å radius, with a clear first “hydration shell,” similar to the first hydration shell in bulk water, and a secondary shell also typically visible. However, oxygen atoms are not the only atoms that can be coordinated by cations, and coordinating atoms for anions are much less well characterized than those for cations. We therefore analyzed all atoms within 6 Å of the cations as well as chloride anions using distance and force-field derived partial charges as criteria to identify atoms that are likely a part of the coordination shells. The code is written in Python and is freely available under the GNU Public License v3 at https://github.com/Becksteinlab/PDB_Ion_Survey

Paul Abers (10)*

Title: Cryogenic Testbed Setup and Testing for Microwave Kinetic Inductance Detectors (MKIDs)
Faculty Mentor: Dr. Phil Mauskopf
Collaborators: Hamdi Mani
Abstract: We designed and constructed a cryostat setup for MKID detectors. The cryostat has four stages: 40K, 4K, 1K and 250mK. The 4K stage is used to cool various devices as well as a stepping stone for further cold stages. It is large enough to mount a few resonator packages, house the sorption cooler and to house the milliKelvin stage. The final stage, 250mK, is designed to house up to a six inch wafer, while being fully enclosed in a radiative shield. A Niobium MKID from Stanford was tested in our cryostat setup for various temperatures and input powers in order to test our system and setup. Lastly, a homodyne noise characterization setup was designed for future testing.

Taylor Colburn (11)*

Title: Simulating the conformational transitions of the transmembrane symporter Mhp1
Faculty Mentor: Dr. Oliver Beckstein
Collaborators: Sean Seyler
Abstract: The function of many proteins depends on large-scale conformational changes. Because these conformational transitions are rare events, it is very difficult to investigate them with equilibrium molecular dynamics (MD) simulations, which have otherwise become an important tool to study the molecular mechanisms of macromolecular systems. A variety of techniques --- such as the Dynamic IMportance Sampling (DIMS) [1] method and various elastic network-based approaches --- have been developed to overcome timescale limitations and produce physically plausible trajectories between putative metastable states. We sought to characterize a number of different path generating and sampling methods, including DIMS with and without an implicit membrane model, by producing multidirectional trajectories of the transmembrane nucleobase symporter Mhp1[2]. All trajectories were compared to one another using Root-Mean-Square Distances (RMSDs), structural order-parameters and Path Similarity Analysis (PSA)[3]. In particular, PSA showed that while trajectory generating methods were broadly similar, paths from each method were also clearly distinguishable.
1. Perilla JR, Beckstein O, Denning EJ, Woolf TB. Computing ensembles of transitions from stable states: Dynamic importance sampling. J Comput Chem. 2011;32(2):196-209.
2. T. Shimamura, S. Weyand, O. Beckstein, N. G. Rutherford, J. M. Hadden, D. Sharples, M. S. P. Sansom, S. Iwata, P. J. F. Henderson, and A. D. Cameron. Molecular basis of alternating access membrane transport by the sodium-hydantoin transporter Mhp1. Science, 328(5977):470–473, 2010. doi: 10.1126/ science.1186303.
3. Seyler SL, Kumar A, Thorpe MF, Beckstein O (2015) Path Similarity Analysis: A Method for Quantifying Macromolecular Pathways. PLoS Comput Biol 11(10): e1004568. doi:10.1371/journal.pcbi.1004568

Thomas Larsen (12)*

Title: Monte Carlo Simulations of Cryo-STEM Tomography
Faculty Mentor: Dr. Peter Rez
Abstract: Scanning transmission electron microscope (STEM) imaging has recently been applied to the cryo-tomography of thick biological specimens. As previously shown for plastic sections, STEM has a number of advantages for cryo-imaging compared to conventional wide-field TEM imaging. STEM is insensitive to phase coherence and is therefore suitable for much thicker specimens than TEM. Imaging in focus, with a long depth of field, also circumvents the complications of an oscillatory contrast transfer function and missing information at low spatial frequencies. Moreover the image signal represents a quantitative measurement of the electron scattering pixel by pixel, so that absolute intensities can be interpreted in terms of material properties in the specimen. Resolution, however, is undoubtedly compromised for thick samples, especially in the regime of multiple elastic scattering. In this work we address the specific issues that arise in cryo-tomography of thick biological specimens. We formulate an imaging model based on a Boltzmann transport equation, complemented by Monte Carlo simulations. Using these theoretical tools, we identify conditions for image acquisition that will be compatible with the basic presumption of tomographic reconstruction, i.e., that for a given composition the imaging signal varies monotonically with thickness. For optimal resolution, contrast, and signal strength, we propose to generalize the on-axis bright field detector to collect at angles well beyond the illumination cone. Our results justify the generation of 3D images for micron thicknesses and beyond.