



Ohio Supercomputer Center

# SUG

## Statewide Users Group

Fall Meeting  
October 6, 2016



**Ohio Supercomputer Center**

An **OH·TECH** Consortium Member

## Flash Talks | 2:15–3:00 pm

### Chemistry (BALE Conference Room)

1. Proximity Effects of Dichalcogenide Monolayers on Graphene  
Abdulrhman Alsharari | Ohio University
2. Surfactant Effectiveness in Ethanol-Water Mixtures  
Phwey (Dan) Gil | Case Western Reserve University
3. Probing the Photodynamics of Rhodopsins with Reduced Retinal Chromophores  
Madushanka Manathunga | Bowling Green State University
4. Strain Fields and Electronic Structure of CrN  
Tomas Rojas Solorzano | Ohio University
5. Effect of Unneutralized Carboxyl Groups on the Behavior of Ionomers from Coarse Grained Molecular Dynamics Simulations  
Janani Sampath | The Ohio State University
6. iSPOT: A Multi-Technique Platform for Structural Modeling of Protein-Protein Complexes  
Sichun Yang | Case Western Reserve University

### Non-Chemistry (BALE Theater)

1. Magnetic Interactions in Novel Two-Dimensional Materials  
Oscar Avalos Ovando | Ohio University
2. Long Short-Term Memory for Speaker Generalization in Supervised Speech Separation  
Jitong Chen | The Ohio State University
3. In the Wake of Dark Giants: New Signatures of Dark Matter Self Interactions in Equal Mass Mergers of Galaxy Clusters  
Stacy Kim | The Ohio State University
4. Speciation with Gene Flow in North American Myotis Bats  
Ariadna Morales | The Ohio State University
5. The Solar Opacity: Large Enhancements in Photoionization and Bound-Free Opacity  
Sultana Nahar | The Ohio State University
6. Pushing the Next-Generation Arctic System Reanalysis to the Human Scale  
Aaron Wilson | The Ohio State University

## Posters : 3:15–5:00 pm

1. A Molecular Study of the Use of Ionic Liquids to Extract the Wastewater Contaminant Atenolol | Miranda Caudle
2. Density Guided MD-Rosetta Protocol for Protein Structure Refinement | Sumudu Leelananda
3. Historical Demography of a Community of Marine Phages Reveals “Killing the Winner” in Action | Sergei Solonenko
4. Valley Polarization in Graphene with Out-of-Plane Deformation | Dawei Zhai
5. Optimizing Genomic Sequencing and Analysis to Detect Microsatellite Instability in Cancer | Esko Kautto
6. Computational Study on Photodynamics of Rhodopsins with Reduced Retinal Chromophores | Xuchun Yang
7. Novel Binding Site of Cyclin A2 and Potential Inhibitors | Stephanie Kim
8. Electron-ion Recombination and Photoionization of P II | Sultana Nahar
9. Study the Interaction of Human Beta Defensin Type 3 with Lipid Membrane | Rabeta Yeasmin
10. Study of Polymer Modified Asphalts Using Molecular Dynamics Simulations | Joshua Berry
11. The Effect of Force Field Selection on Modeling Binary Aqueous Mixtures | Garrett Long
12. Evaporation of Water in Hydrophobic Confinement | Mohsen Ghasemi
13. Shear Viscosity Prediction of Pure Molecules Using Molecular Dynamic Method | (Tessa) Tyler Eskander
14. A First-Principles Study of Defects in Ni-Based Alloys | You Rao
15. Modeling Crystal Structure Using Magnetic Ising Model | Patrick Gemperline
16. Modeling the Effects of Yttrium Solutes on  $\langle c+a \rangle$  Dislocations in Mg | Daniel Buey
17. Finite-Difference Time-Domain (FDTD) Modeling of Liposome-Based Substrates for Surface-Enhanced Raman Spectroscopy (SERS) | Zohre Gorunmez
18. Slip-Stimulated Twinning Across Grain Boundaries in Titanium | Mohammad Shahriar
19. Which Clouds are Important: Variation of Cloud Size Distribution Functions in Large Eddy Simulations | Dorothy Pharis
20. Determination of Domain Spacing in Double Gyroid Phase of Pure Diblock Copolymers | Kuan-Hsuen Shen
21. Ab Initio Study on Point Defects in Cubic Boron Arsenide (BAs) | Yaxian Wang
22. An Ab Initio Method for Improving Atom Probe Tomography Simulations | Travis Withrow
23. Developing Novel Techniques for Searching for Ultra-High Energy Neutrinos in Antarctic Ice at OSC | Amy Connolly
24. On the Distribution of Humidity in the Convective Atmospheric Boundary Layer | Robert White
25. Computationally Guided Resonance Raman Spectroscopy of Nickel-Substituted Rubredoxin, A Model Hydrogenase Enzyme | Sean Marguet
26. Combining MOSCED with Electronic Structure Calculations to Develop an Efficient Tool for Solvent Formulation and Selection | Andrew Paluch
27. Improved Atmospheric De-Aliasing Product for Satellite Gravimetry | Yu Zhang