Ohio Supercomputer Center

SUG

Statewide Users Group

Fall Meeting
October 6, 2016

Ohio Supercomputer Center
An OH·TECH Consortium Member

Agenda

Thursday, October 6

9:00–10:00 am	Q&A with OSC Help	BALE Conference Room
10:00–11:00 am	Software and Activities Committee Hardware and Operations Committee OSC Help: Available	Buckeye Room Csuri Room BALE Conference Room
11:00–11:15am	**Break**	
11:15 am–12:00 pm	Industrial Keynote: Duane Detwiler	BALE Theater
12:00–12:15 pm	**Lunch Pick-up**	**BALE Theater**
12:15–1:15 pm	OSC Presentation (food welcome)	BALE Theater
1:15–2:00 pm	Academic Keynote: Alexey T. Zayak	BALE Theater
2:00–2:15 pm	**Break**	
2:15–3:00 pm	Chemistry Flash Talk Session Non-Chemistry Flash Talk Session	BALE Conference Room BALE Theater
3:00–3:15 pm	**Break**	
3:15–5:00 pm	Poster Session Begins Social Networking OSC Help: Available	BALE Area BALE Area BALE Conference Room
5:00 pm	Poster and Flash Talk Winner Announcement	BALE Area

Keynote Addresses

11:15 am–12:00 pm

Duane Detwiler

Chief Engineer of Vehicle Research and Manager of the Strategic Research Department at Honda R&D Americas, Inc.

CAE for Lightweight Vehicle Development

The automotive industry shares the goal to develop advanced vehicle structures which are light weight yet perform well for a variety of performance criteria without incurring significant penalties to manufacturing costs or efficiency. In order to further improve the efficiency of our development process and the quality of our products Honda has increased our ability to predict performance for a given vehicle design using Computer Aided Engineering. This presentation will highlight current CAE methods used for virtual validation of vehicle designs and consider computational challenges for future greater application of lightweight materials and technologies.

1:15–2:00 pm

Alexey T. Zayak

Assistant Professor of Physics and Astronomy at Bowling Green State University

Computational angle to vibrational spectroscopy of heterogeneous chemical interfaces

Raman spectroscopy promises exciting opportunities, able to report about a particular chemical species and its interaction with the immediate chemical environment. It utilizes interactions of light with atomic vibrations and provides unique "fingerprints" of any chemical species. While the conventional Raman spectroscopy cannot be used at the nano-scale due to its extremely small scattering cross section and the far-field diffraction limit of light, the Surface Enhanced Raman Spectroscopy (SERS) has emerged to overcome these weaknesses. In this talk, I will give a brief overview of SERS and focus on the chemical aspect of this phenomenon to demonstrate how Raman interactions can reveal local chemical interactions, visualizing the role of the interfacial electron-phonon coupling. Our results obtained using Oakley demonstrate unique capabilities of the Raman scattering for studying interfacial properties.

Flash Talks | 2:15–3:00 pm

Chemistry (BALE Conference Room)

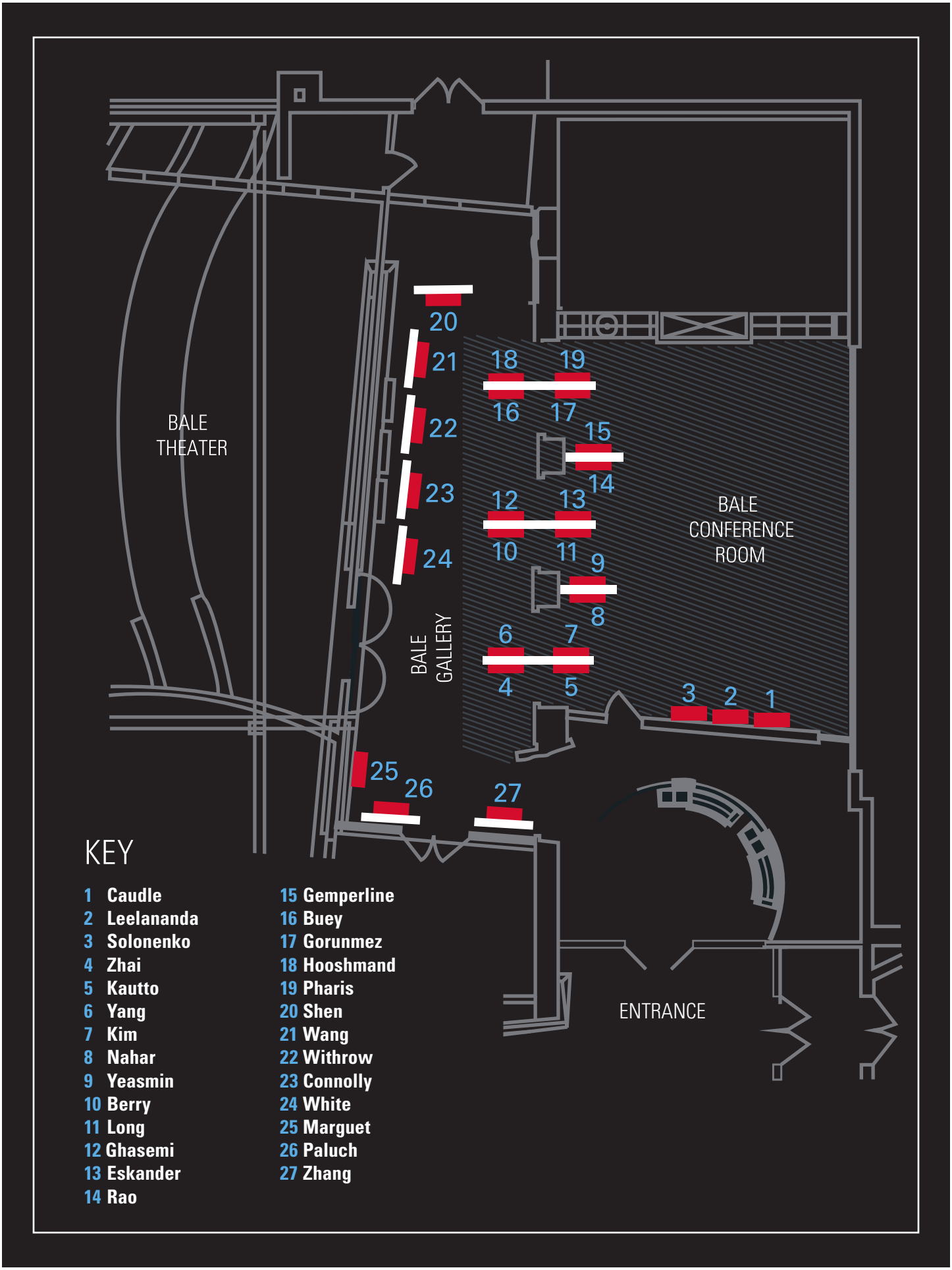
1. Proximity Effects of Dichalcogenide Monolayers on Graphene
   Abdulrhman Alsharari | Ohio University
2. Surfactant Effectiveness in Ethanol-Water Mixtures
   Phwey (Dan) Gil | Case Western Reserve University
3. Probing the Photodynamics of Rhodopsins with Reduced Retinal Chromophores
   Madushanka 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

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 <c+a> 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-Hsuan 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



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