



**LLNL - UC Davis Electronic Structure Workshop**  
**QSG – Angstrom – Electronic Structure Laboratory**  
**Lawrence Livermore National Laboratory**  
**October 20-21, 2011**

**Day 1 – Thursday, October 20, 2011**

6:30 PM	<i>Dinner + poster session</i>	
9:00 AM	<i>Arrive at Badge Office</i>	
10:00 AM	<i>NIF Tour</i>	
12:00-1:15 PM	<i>Working lunch, B319</i>	Giulia/Francois/Eric
1:15 PM	<i>Move to HPCIC, T6474</i>	
1:30-1:50 PM	Optical absorption spectra: overview of techniques to solve the Bethe Salpeter Equation	Dario Rocca
1:50-2:10 PM	Explicit integrators for time-dependent Kohn-Sham equations	Andre Schleife
2:10-2:30 PM	Photoemission spectra and electronic gaps: Many body perturbation theory (GW) overview	Tuan Anh Pham
2:30-2:50 PM	QMC/PIMC	Jonathan DuBois
2:40-3:10 PM	<i>Break</i>	
3:10-3:30 PM	All-electron versus pseudopotential calculations of electronic screening	Amandeep Kaur
3:30-3:50 PM	Ab-initio Md on GPUs	William D. Dawson
3:50-4:10 PM	van der Waals functionals	Jun Wu
4:10-4:30 PM	ESTEST framework	Gary Yuan
4:30-4:50 PM	<i>Break</i>	
4:50-5:10 PM	MD simulations of thermal transport: nano-wires and nanoporous Si and Ge	Yuping He
5:10-5:30 PM	Atomistic heat transport in nanowire devices	Davide Donadio
5:30-5:50 PM	Boltzman transport treatment of heat transport in mass disordered systems	Ivana Savic

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## Day 2 – Friday, October 21, 2011

Time	Description	Presenter
8:30 AM	<i>Arrive at HPCIC, T6474</i>	
8:40-9:00 AM	Overview of ab-initio MD simulations of water	Cui Zhang
9:00-9:20 AM	Ionic quantum effects in water at ambient conditions	Miguel Morales
9:20-9:40 AM	Ice at low and high P: interplay between hydrogen bonding and vdW interactions	Eamonn Murray
9:40-10:00 AM	Complex mixtures under pressure	Sebastien Hamel
10:00-10:20 AM	<i>Break</i>	
10:20-10:40 AM	High pressure water and mixtures	Ding Pan
10:40-11:00 AM	Pristine Methane and methane on surface, under the Earth mantle conditions	Leonardo Spanu
11:00-11:20 AM	Hydrogen equation of state	Alfredo Correa
11:20-11:40 AM	H <sub>2</sub> O/H <sub>2</sub> SO <sub>4</sub> liquid mixtures	Quan (Andy) Wan
12:00-1:30 PM	<i>Lunch offsite</i>	
2:00-2:20 PM	Predictive modeling of defect properties of materials for radiation detection and quantum computing	Vince Lordi
2:20-2:40 PM	Simultaneously tuning the electronic and ionic properties of TlBr	Cedric Rocha Leao
2:40-3:00 PM	Intel materials overview	Sadasivan Shankar
3:00-3:20 PM	Boron	Tadashi Ogitsu
3:20-3:40 PM	<i>Break</i>	
3:40-4:00 PM	PEC	Brandon Wood
4:00-4:20 PM	Doped WO <sub>3</sub> and Caltech project	Yuan Ping
4:20-4:40 PM	Multi exciton generation (MEG) for solar cells	Marton Voros
4:40-5:00 PM	Solar project: looking for MEGs	Stefan Wippermann
5:00-5:20 PM	Wrap up	