ES2015 Meeting Program

SUNDAY, JUNE 21, 2015		
11:00 AM	Early check-in approved for all ES2015 participants	Lander Hall
12:30 PM-4:00 PM	ES2015 Coordinator: conference materials & guides	ES2015 desk at Lander Hall
6:00 PM-8:00 PM	Informal gathering for dinner/drinks near the Ave	Alder Hall Lounge enter from NE Campus Parkway

MONDAY, JUNE 22, 2015 *Scientific Program (Haggett Hall, Cascade Room)*		
8:30 AM-8:40 AM	**Opening Remarks**	
Session Chair: David Vanderbilt		***New Methods***
8:40 AM-9:10 AM	Jim Chelikowsky, U of Texas, Austin	*"Seeing" the covalent bond: Simulating Atomic Force Microscopy Images*
9:10 AM-9:22 AM	Alexandru Bogdan Georgescu, Yale	*A Generalized Slave-Particle Formalism for Extended Hubbard Models*
9:22 AM-9:52 AM	Bryan Clark, U of Illinois, Urbana Champaign	*From ab-initio to model systems: tales of unusual conductivity in electronic systems at high temperatures*
9:55 AM-11:10 AM	**Poster Session A // Coffee Break**	
Session Chair: Natalie Holzwarth		***Advances in DFT and Applications***
11:10 AM-11:40 AM	Priya Gopal, Central Michigan U	*Novel tools for accelerated materials discovery in the AFLOWLIB.ORG repository: breakthroughs and challenges in the mapping of the materials genome*
11:40 AM-11:52 AM	Ismaila Dabo, Penn State U	*Electronic-Structure Calculations from Koopmans-Compliant Functionals*
11:52 AM-12:22 PM	Eric Bylaska, PNNL	*Improving the performance of ab initio molecular dynamics simulations and band structure calculations for actinide and geochemical systems with new algorithms and new machines*
12:25 PM-1:40 PM	**Free time for lunch**	**(Debit dining cards provided to West Campus Dorm guests accepted at McMahon 8, Ian's Domain and the Hub)**
Session Chair: George Bertsch		***QMC***
1:40 PM-2:10 PM	Hao Shi, College of William & Mary	*Recent developments in auxiliary-field quantum Monte Carlo: magnetic orders and spin-orbit coupling*
2:10 PM-2:22 PM	Fengjie Ma, College of William and Mary	*Ground and excited state calculations of auxiliary-field Quantum Monte Carlo in solids*
2:22 PM-2:52 PM	Paul Kent, ORNL	*New applications of Diffusion Quantum Monte Carlo*
2:52 PM-4:07 PM	**Poster Session B // Coffee Break**	
Session Chair: Andrew Rappe		***Many Body***
4:07 PM-4:37 PM	Diana Qiu, UC Berkeley	*Many-body effects on the electronic and optical properties of quasi-two-dimensional materials*
4:37 PM-4:49 PM	Mei-Yin Chou, Academia Sinica	*Dirac Electrons in Silicene on Ag(111): Do they exist?*
4:49 PM-5:19 PM	Emmanuel Gull, U of Michigan	*Solutions of the Two Dimensional Hubbard Model: Benchmarks and Results from a Wide Range of Numerical Algorithms*
5:20 PM	**Free evening in town**	
5:40 PM	**Optional Tutorial open-source RMG code for electronic structure calculations**	

TUESDAY, JUNE 23, 2015 *Scientific Program (Haggett Hall, Cascade Room)*		
Session Chair: Jerry Bernholc		***Dynamics***
8:30 AM-9:00 AM	David Prendergast, LBNL	*First-principles explorations of dynamics in materials - from attoseconds to nanoseconds - aided by X-ray spectroscopy*
9:00 AM-9:12 AM	Shuai Zhang, UC Berkeley	*Superionic water at planet interior |an ab initio molecular dynamics study*
9:12 AM-9:42 AM	Jean-Luc Fattebert, LLNL	*Truly Scalable O(N) Approach for First-Principles Molecular Dynamics of Non-Metallic Systems*
9:45 AM-10:15 AM	**Coffee Break**	
Session Chair: David Ceperley		***Ultra-fast and Energy-related***
10:15 AM-10:45 AM	Marco Bernardi, UC Berkeley	*Ultrafast Dynamics of Excited Electrons in Semiconductors and Metals for Energy Applications*
10:45 AM-10:57 AM	Kyle Reeves, UNC, Chapel Hill	*First-Principles Investigation of Electronic Excitation Dynamics in Water under Proton Irradiation*
10:57 AM-11:27 AM	Alexie Kolpak, MIT	*First-principles prediction of oxide surface structure and properties in aqueous electrochemical environments*
11:30 AM-1:00 PM	**Free time for lunch**	**(Debit dining cards provided to West Campus Dorm guests accepted at McMahon 8, Ian's Domain and the Hub)**
Session Chair: John Rehr		***Finite Temp and Magnetic Fields***
1:00 PM-1:30 PM	Sam Trickey, U of Florida	*Finite-temperature Density Functional Developments and Some Computational Consequences*
1:30 PM-1:42 PM	Bruce Harmon, Iowa State University	*LaCoO3 (LCO): electronic structure changes at very high magnetic fields - up to 500T*
1:42 PM-2:12 PM	Michel Côté, Université de Montréal	*Electron-phonon coupling and the zero-point phonon renormalization of the electronic band gap*
2:15 PM-2:45 PM	**Coffee Break**	
Session Chair: Richard Martin		***TDDFT***
2:45 PM-3:15 PM	George Bertsch, U of Washington	*Time-dependent Density Functional Theory in the Nonlinear Domain: Successes and Failures*
3:15 PM-3:27 PM	Grigory Kolesov, Harvard U	*Time-dependent density functional theory and non-adiabatic Ehrenfest dynamics with localized basis sets : method and applications*
2:37 PM-3:57 PM	Neepa Maitra, Hunter College	*Potentials that Exactly Capture Correlated Electron and Ion Dynamics in Strong Fields*
3:57 PM- 4:27 PM	Xiaosong Li, U of Washington	*Time-Dependent Two-Component Electronic Structure Theory*
6:30 PM-9:00 PM	**Banquet at Ivar's Salmon House**	**401 NE Northlake Way, Seattle, WA 98105**

WEDNESDAY, JUNE 24, 2015 *Scientific Program (Haggett Hall, Cascade Room)*		
8:30 AM-8:45 AM	**CEI Poster Awards**	
Session Chair: Roberto Car		***Green's Functions***
8:45 AM-9:15 AM	Lucia Reining, Ecole Polytechnique	*A direct approach to the calculation of many-body Green's functions*
9:15 AM-9:27 AM	Wenchang Lu, North Carolina State U	*Ab initio non-equilibrium Green's function studies of electronic devices with several thousand atoms*
9:27 AM-9:57 AM	Joshua Kas, U of Washington	*Cumulant expansion approaches to excited state electronic structure and spectra*
10:00 AM-10:30 AM	**Coffee Break**	
Session Chair: Mei-Yin Chou		***GW-BSE***
10:30 AM-11:00 AM	Linda Hung, U of Illinois, Chicago	*GW-BSE: From Atoms to the Nanoscale*
11:00 AM-11:12 AM	John Vinson, NIST	*Using RIXS to probe effects of disorder and quasiparticle lifetime broadening*
11:12 AM-11:42 AM	Feliciano Giustino, U of Oxford	*Band structure of plasmonic polarons using the Sternheimer-GW method*
11:45 AM-11:55 AM	**Closing Remarks**	