

Presentation Schedule

9:30am	Poul Jorgensen, "Towards a blackbox optimization of the Hartree-Fock and Kohn-Sham energy"
9:50am	Ken Jordan, "Application of a Drude Model to Excess Electron-Water Cluster Systems"
10:10am	Ron Shepard, "A Graphical Based Nonlinear Wave Function Expansion"
10:30am	Doug O'Neal, "Programming for large Beowulf clusters or multi-processor SGI linux systems"
10:50am	BREAK
11:10am	Ricky Kendall, "TBD"
11:30am	Peter Schmidt, "TBD"
11:50am	Maciek Gutowski, "Designing materials for hydrogen storage"
12:10am	Ramon Hernandez, "Spin-orbit coupling in O ₂ (v) + O ₂ collisions: a new energy transfer mechanism"
12:30 (noon)	LUNCH
2:00pm	Alex Boldyrev, "Advancement of Chemical Bonding Concepts: Then and Now"
2:20pm	Vince Ortiz "TBD"
2:40pm	Mike Salazar, "Toward Molecular Dynamic Simulations of Complex Gas-Phase Reactive Systems on Ab Initio PESs"
3:00pm	Lai-Sheng Wang, "Multiply Charged Anions"
3:20pm	BREAK
3:40pm	Tony Haymet, "Nucleation"
4:00pm	Robert Gdanitz, "Accurately solving the electronic Schrödinger equation of small atoms and molecules using explicitly correlated (r_{12} -)MR-ACPF: Valence excited states of methylene (CH ₂)."
4:20pm	Jacek Jakowski, "Mixed ab initio and quantum wavepacket dynamics"
4:40pm	Orville Day, "Black Holes – The Hydrogen Atoms of Astrophysics"
5:00pm	Conclusion