Many Body Interactions: From Quantum Mechanics to Force Fields
Presentation Titles

Christian	Burnham	Modeling the Proton Potential in water. What are the Spectroscopic Data
David	Case	Biomolecular Force Fields Using Implicit Solvation
Tom	Darden	Fast Reciprocal Space Based Methods for Coulomb Integrals
Albert	DeFusco	Many-Body Effects in Water Clusters
Alexander	Donchev	
J. Daniel	Gezelter	Many-Body Effects in Metal-Water Interactions
Ian	Hamilton	Many-Body Effects for Small Clusters of Metallic (Gold) and Covalent (Carbon) Atoms
Teresa	Head-Gordon	Structure and Dynamics of Disease Peptides from the Interplay of NMR Experiments and Molecular Simulations: Challenges for Force Fields and Sampling
Jan	Jensen	EFP/FMO: Blurring the QM/MM Boundary
Frank	Jensen	Force Field Conformational Energies
Ken	Jordan	Use of Model Hamiltonian Approaches for Describing Excess Electrons in Water
Gunnar	Karlstrom	Modeling of the Molecular Charge Reorganization Induced by Variation of Dihedral Angles
Kozuo	Kitaura	Electronic Structure Calculations of Proteins Using the Fragment Molecular Orbital Method
John	Klepeis	Development of Molecular Mechanics Force Fields for Long-time Scale Molecular Dynamics Simulations
Revati	Kumar	A Modified MSEVB Approach for Modeling Excess Protons in Water
Hui	Li	Modeling Exchange-Repulsion, Electrostatic, and Polarization
Alston	Misquitta	Recent Developments in *Ab Initio* Methods for Molecular Interactions:Atom-Atom potentials for the Condensed Phase
Kim	Palmo	
Jean-Philip	Piquemal	Toward Quantitative Molelcular Modeling: Development of Quantum Chemistry Tools and New Generations of Force Fields
Julia	Rice	Do We Need to Include Higher Order Terms in Periodic Ewald QM/MM Calculations? Comparison of Classical and QM/MM Potentials for the Potential of Mean Force for Rotation Around an Amide Bond
Ulf	Ryde	Accurate Free Energies in Proteins with a Combination of QM and MM Methods
David	Sherrill	Comparing Force Fields to Benchmark-Quality *Ab Initio* Data for Noncovalent Interactions

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Lyudmilla	Slipchanko	Forces that Govern Life: On the Way to Understanding Intermolecular Interactions
Anthony	Stone	Putting the Induction Energy into Many-Body Force Fields
Bill	Swope	Benefits of Using QM/MM Techniques to Evaluate and Improve Force Fields
John	Thomas	Water Flow Through Carbon Nanotubes and the Water/Carbon Nanotube Interaction Potential
Krysztof	Szalewicz	How Accurate can be Intermolecular Potentials and Who Cares
Piet	van Duijnen	The Discrete Reaction Field Approach to QM/MM
Darrin	York	Progress Toward a Next Generation Quantum Force Field for Molecular Simulations

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