Tentative Schedule for the
Telluride Workshop on Many-Body Interactions:
From Quantum Mechanics to Force Fields

Organizers: Kenneth Jordan and Jean Philip Piquemal
TSRC Hosts: Nana Naisbitt 970-708-0004 and Rory Sullivan 970-708-4542
Dates: June 15-19, 2014

Saturday Evening
6:00-8:00PM Informal "Meet & Greet" at Arroyo Wine Bar & Gallery, 220 E. Colorado (Main St.), cash bar

Sunday Morning, June 15th

7:30-8:00AM	Breakfast at TSRC		
8:00-8:10AM	Opening Remarks		
8:10-8:50AM	F1	David Sherrill	Comparing Force Fields to High-Accuracy Coupled-Cluster Theory and Symmetry-Adapted Perturbation Theory
8:50-9:30AM	F2	Yiman Wang	*Ab Initio* Many-Body Potentials for Water and Ion Hydration
9:30-9:50AM	S1	Eugene Kamarchik	Many-Body Approach to Vibrational Calculations
9:50-10:10AM	Coffee Break		
10:10-10:50AM	F3	Mike Gillan	Energy Benchmarking of Liquids and Solids with Quantum Monte Carlo
10:50-11:30AM	F4	Gabor Csanyi	Reactive Many-Body Expansion
11:30-11:50AM	S2	Alan Nichol	Automatic Fitting of Intra- and Intermolecular Potentials with GAP
11:50AM-12:10PM	S3	Omar Demerdash	Improving the Computational Efficiency of the Induced-Dipole Model in the AMOEBA force Field via the 3-Body Approximation: Algorithmic Development and Validation on Condensed-Phase Properties of Water

Sunday Evening, June 15th

7:00-7:40PM	F5	Ken Jordan	Model Hamiltonians for Describing Excess Electron Systems
7:40-8:20PM	F6	Gregory Beran	Low-Cost Electronic Structure Approaches for Intermolecular Interactions: From Dimers to Crystals
8:20-8:40PM	S4	Lee-Ping Wang	Building a compromise between experiment and ab initio theory in effective pair potentials

Monday Morning, June 16th

7:30-8:00AM	Breakfast at TSRC		

8:00-8:40AM	F7	Glen Martyna	The Quantum Drude Oscillator Model : A Non-Perturbative and Unified Treatment of Many Body Polarization
8:40-9:20AM	F8	Alexandre Tkatchenko	Unexpected Aspects of Many-Body Dispersion Interactions
9:20-9:40AM	S5	Alexander Donchev	Improved Accuracy in the Modeling of Dispersion Interactions for MD simulations
9:40-10:00AM Coffee Break			
10:00-10:40AM	F10	Jay Ponder	Recent Improvements to the AMOEBA Force Field
10:40-11:20AM	F11	Filippo Lipparini	Polarizable Molecular Dynamics in a Polarizable Continuum Solvent: Is This Possible?
11:20-12:00AM	F12	Markus Meuwly	Multipolar Electrostatics and Its Applications in Atomistic Simulations

Monday Evening, June 16th

5:30-7:15PM	Workshop Dinner		Rustico, 114 E. Colorado (Main) Reservation pending
7:40-8:20PM	F13	Leim Dang	Computational Studies of Ions Solvation with Ring Polymer Molecular Dynamics
8:20-8:40PM	S6	Leonid Pereyaslavets	Systematic Errors in Hydration Free Energies Calculated with Classical and Polarizable Force Fields

Tuesday Morning, June 17th

7:30-8:00AM	Breakfast at TSRC		
8:00-8:40AM	F14	Pär Söderhjelm	Comparison between Simple and Advanced Force Fields in Calculating Hydration Free Energies
8:40-9:20AM	F15	Seymour Wang	MP2 Solvation Free Energies of Ions from Adaptive Force Matching
9:20-9:40AM	S7	Jan Steckel	Force Matching in the Condensed Phase
9:40-10:00AM Coffee Break			
10:00-10:40AM	F16	Andres Cisneros	Development of Advanced Polarizable Force Fields for Water and Ionic Liquids
10:40-11:00AM	S8	Julia Rice	How to use quantum mechanics to derive a fixed charge force field for molecular simulation
11:00-11:20	S9	Bill Swope	How to match fixed charge force fields with more exact representations
11:20-12:00PM	F17	Francesco Paesani	Water Potential with Chemical Accuracy for Simulations From the Gas to the Condensed Phase

Tuesday Evening, June 17th

6:00-9:00PM Traditional TSRC Picnic @ Telluride Intermediate/High School Soccer Field

Wednesday Morning, June 18th

7:30-8:00AM Breakfast at TSRC

8:00-8:40AM	F18	David Case	Adventures with Simple, Fixed-Charge Force Fields for Proteins
8:40-9:20AM	F19	Louis Vanduyfhuys	QuickFF: Toward a Generally Applicable Methodology to Quickly Drive Accurate Force Fields for Metal-Organic Frameworks from Ab Initio Input
9:20-9:40AM	S10	Karl Debiec	Are Salt Bridges Overstabilized? A Comparison of Current biomolecular Force Fields

9:40-10:00AM Coffee Break

10:00-10:40AM	F20	Brian Space	Polarizable potentials for MOF sorption that work (or don't)
10:40-11:20AM	F21	Laura Gagliardi	Quantum Chemically Derived Force Fields for Gas Separations in Metal-Organic Frameworks
11:20-12:00PM	F22	Paul Popelier	Quantum Chemical Topology for Biomolecular Simulation

Wednesday Evening, June 18th

7:00-7:40PM	F23	Mike Schneiders	Many-Body Algorithms for Crystal Thermodynamics and Protein Structure Refinement
7:40-8:00PM	S11	Jean-Philip Piquemal	Accelerating Polarizable Molecular Dynamics: New Algorithmic for Massively Parallel Simulations
8:00-8:20PM	S12	Christopher Narth	Porting SIBFA into Tinker
8:20-8:40PM	S13	Odbadrakh Tuguldur	n-BODY Interactions in Gas Hydrates