Schedule for the Telluride Workshop on Many-Body Interactions from Quantum Mechanics to Force Fields

Monday Morning

7:30-8:00	Breakfast at the meeting site	
8:00-8:10	Opening Remarks	
8:10-8:50	Ken Jordan	"Incorporating Electron Correlation Effects in Electron-Water Interactions via Model Potentials"
8:50-9:30	Teresa Head-Gordon	"iAMOEBA: a direct polarization model"
9:30-9:50	Lori Burns	"Assessing the Performance of Density Functional and Wavefunction Methods for Noncovalent Interactions"
9:50-10:10	Break	
10:10-10:50	Alston Misquitta	"The role of Explicit Polarization on the Energy Landscape of Pyridine Clusters"
10:50-11:30	Greg Schenter	"EXAFS Analysis of Molecular Interaction"
11:30-11:50	Jan Steckel	"Electronic Structure Calculations of the Acetate-CO_2 Interaction: Implications for Force Field Development"
11:50-12:10	Open Discussion	

Monday Evening

7:00-7:40	Susan Sinnot	"Charge Optimized Many-Body (COMB) Potentials: Development and Applications"
7:40-8:20	Carsten Mueller	"Electron Correlation Effects in Extended Systems"

Tuesday Morning

7:30-8:00	Breakfast at the meeting site	

8:00-8:40	Jay Ponder	"The AMOEBA Force Field: Current Problems and Possible Solutions"
8:40-9:20	Andreas Cisneros	"Use of Gaussian Electrostatic Model Distributed Multipoles in AMOEBA"
9:20-9:40	Fangfang Wang	"DPP2 and DPP3 Water Models"
9:40-10:00	Break	
10:00-10:40	David Sherrill	"The Importance of Charge Penetration of Pi-Interactions"
10:40-11:20	Gary Kedziora	"DFT molecular dynamics: from validation to simulation"
11:20-11:40	Aude Marjolin	"Modeling of Lanthanide and Actinide Cations: From QM to MM"
11:40-12:00	Open Discussion	

Tuesday Evening

6:00 - 7:15 p.m., Town Talks at the Palm Theatre

"Learning from Nature's 3-Billion-Year Solar Energy Program," Gregory Scholes, University of Toronto

"Plastic Solar Cells: Learning how molecule think," Peter Rossky, Departments of Chemistry and Chemical Engineering, University of Texas at Austin

7:30-8:10	Carine Clavaguera	"IR Spectroscopy of Gas Phase and Micro-Hydrated Biolmolecules with New Generation Force Fields"
8:10-8:30	A. Donchev/John Klepeis	"Polarizable Force Field Development at D. E. Shaw"

Wednesday Morning

7:30-8:00	Breakfast at the meeting site	
8:00-8:40	Liem Dang	"Understanding Ion-Ion Interactions in Bulk and Aqueous Interfaces Using Molecular

		Simulations"
8:40-9:20	Jiali Gao	"Variational Many-body Expansion in the Framework of Block-Localization"
9:20-9:40	Karl Diebec	"Atomistic Simulations of a Two-Domain Protein on the Microsecond Time-Scale"
9:40-10:00	Break	
10:00-10:40	Gabor Csanyi	"A Systematic Bayesian Approach to Potentials"
10:40-11:20	Jean-Philip Piquemal	"Improving polarizable force fields: from small energy differences to free energies."
11:20-11:40	Mike Schnieders	"Accelerating Polarizable Multipole AMOEBA Free Energy Calculations Using Orthogonal Space Methods"
11:40-12:00	Open Discussion	

Wednesday Evening

5:00-7:00	Workshop dinner at Floradora	
7:20-8:00	Nohad Gresh	"Development, Validation, Applications, and Perspectives of Polarizable, Anisotropic Molecular Mechanics Potentials"
8:00-8:40	Laura Gagliardi	"Bridging the Gap between Quantum Chemistry and Classical Simulations for CO_2"

Thursday Morning

7:30-8:00	Breakfast at the meeting site	
8:00-8:40	Feng Wang	"Investigating the Free Energy of Ice and Water on a Coupled Cluster Quality Potential Energy Surface through a Force Field"
8:40-9:20	Pengyu Ren	"Development of Polarizable Multipole Force Field and its Applications"

9:20-9:40	Break	
9:40-10:20	Alexander Tkatchenko	"Accurate and Efficient First-Principles Calculation of van der Waals Energy"
10:20-11:00	Robert DiStasio	"Many-Body van der Waals Interactions: Theory and Applications"
11:00-11:40	Jean-Pierre Dognon	"f-Elements Theoretical Chemistry: From Structure to Thermodynamics"
11:40-12:00	Open Discussion	

Thursday Evening

6:00-9:00 Picnic

Friday Morning

Departure