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Frontiers in Materials Science and
Advanced Computing, Mathematics, and Data
Seminar Series

Advanced Potential Energy Surfaces for Condensed Phase Simulation

Teresa Head-Gordon
Professor, UC Berkeley
Scientist, Lawrence Berkeley National Laboratory

January 26, 2015
10-11 a.m.
ETB Columbia River Room

In her talk, Dr. Head-Gordon will introduce new theoretical models and methods that include direct and mutual polarization based on the AMOEBA (atomic multipole optimized energetics for biomolecular applications) polarizable force field and a Poisson-Boltzmann semi-analytic method. These models and their implementations on multicores are opening new abilities to allow larger scales of study for molecular simulation with more complex potential energy surfaces.

Dr. Head-Gordon is a professor at UC Berkeley in the departments of Chemistry, Bioengineering, and Chemical and Biomolecular Engineering, and a scientist at the Lawrence Berkeley National Laboratory. Her research program focuses on the interface of theoretical chemistry with biology and physics.

Hosted by:
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