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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.

A professor at UC Berkeley and scientist at Lawrence Berkeley National Laboratory since 1992, Dr. Head-Gordon also serves as a faculty staff scientist at the California Institute for Quantitative Biosciences and at Clare Hall, Cambridge, United Kingdom. She has received the IBM Shared University Research (SUR) Award in 2001 and served as the Schlumberger Professor, Cambridge University, United Kingdom in 2005-2006. Dr. Head-Gordon was a panel member of the U.S. National Academies Study on potential impact of advances in high-end computing in science and engineering in 2006-2007 and of the National Institutes of Health Study Section on Modeling and Analysis of Biological Systems in 2007-2012. Her service on editorial advisory boards includes the *Journal of Computational Chemistry* (2004-present), the *Journal of Physical Chemistry B* (2009-2011), and the Society for Industrial and Applied Mathematics (SIAM) book series on Computational Science and Engineering (2004-2009). She was the editor for *Biophysical Journal* in 2003-2006.

Dr. Head-Gordon received a B.S. in Chemistry from Case Western Reserve University in 1983, and a Ph.D. in Theoretical Chemistry from Carnegie Mellon University in 1989. She was a postdoctoral member of the technical staff at AT&T Bell Laboratories from 1990-1992.

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