CHEMICAL ENGINEERING

SEMINAR SERIES

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The role of an accurate description of local structure to inform our understanding of nucleation and assembly

ABSTRACT: A challenge in materials science is how to utilize information from a molecular simulation to build a quantitative model of nucleation and assembly. I will make the case that an accurate description of local structure, as verified by experiment, is imperative in order to describe long-range collective response.

We use the tools of statistical mechanics and molecular simulation (classical and quantum) to construct reduced models of interaction based on the principle of solvent response to interfaces. Thus, providing a link from molecular scale descriptors to macroscopic outcomes.

RECEPTION 3:30 • LECTURE 4:00 – 5:00
PHYSICS ASTRONOMY BLDG. (PAA) A110

CHEMICAL ENGINEERING
UNIVERSITY of WASHINGTON
Knowledge and solutions for a changing world

BIOGRAPHY:

Professional Interests: Equilibrium and non-equilibrium statistical mechanics; *Ab initio* and classical molecular dynamics development and applications; Large-scale *ab initio* computer simulations

Education and Employment

2016-present Affiliate Professor, Department of Chemical Engineering, UW

2006-present Chief Scientist, Molecular Interactions & Transformation, Physical Sciences Division, Pacific Northwest National Laboratory, Richland, WA

2005-2006 Group Leader, Computational Chemistry and Chemical Biology, Lawrence Livermore National Laboratory, Livermore, CA

2003-2004 Deputy Scientific Capabilities Leader, Computational Chemistry and Chemical Biology, Lawrence Livermore National Laboratory, Livermore, CA

2001-2003 Technical Staff, Lawrence Livermore National Laboratory, Livermore, CA

2000-2001 Technical Staff, Sandia National Laboratories, Livermore, CA

1998-2000 Post-doctoral Fellow (Michele Parrinello), Max-Planck-Institut fuer Festkoerperforschung, Germany

1993-1998 Post-doctoral Fellow (Michael L. Klein), Center for Molecular Modeling, University of Pennsylvania

1992 Ph.D., Physical Chemistry (Kenneth Dawson), University of California, Berkeley

1988 B.S. (Hon.), Chemistry, Montana State University, Bozeman, MT

Professional Affiliations

American Chemical Society

American Physical Society

Awards

Fellow of the American Physical Society (2014)

Relevant Publications:

See http://scholar.google.com/citations?user=-MpNANoAAAAJ&hl=en for all publications