

Nanoporous Materials Genome Center Kick Off Meeting

November 17 & 18, 2012 | University of Minnesota

Location: University of Minnesota
Campus Club, Conference Rooms A, B, C
4th Floor Coffman Memorial Union
300 Washington Avenue SE
Minneapolis, MN 55455
www.campusclubmn.org

Hotel Info: Aloft Minneapolis
900 Washington Avenue South
Minneapolis, MN 55415
Phone: 612-455-8400
alofthotels.com/minneapolis

Shuttle Info: Total Transportation
phone: 651-770-5668/651-604-8903
Shuttle will pick up/drop off at the same locations of the lobby of the Aloft Hotel and the East River Road Entrance of Coffman Memorial Union. Take Coffman Union Elevators to the 4th floor, Campus Club. There will be signage directing you to conference rooms A, B, C.

Taxi Info: If you are leaving the meeting early the Campus Club on-sight manager can assist you with arranging taxi service.

For emergency assistance Danell Garber can be reached on her cell phone at 651-247-9730.

Saturday, November 17, 2012

Campus Club, 4th Floor Coffman Memorial Union, Conference Room A & B

Time	Topic	Speaker
8:30 am	Shuttle will depart Aloft Hotel for Coffman Memorial Union	
9:00 am	Opening statements and Overview of the Center	Laura Gagliardi
9:20 am	BES Program Officer	Mark Pederson
9:40 am	Administrative and Managing Director	Danell Garber
9:50 am	Overview of Thrust 1	Laura Gagliardi
10:00 am	Overview of Thrust 2	Berend Smit
10:10 am	Break	
10:30 am	Experimental Context	Jeff Long & Joe Hupp
11:00 am	Washington State University	Aurora Clark
11:10 am	University of Minnesota	Chris Cramer, Ilja Siepmann, Don Truhlar, Michael Tsaptsis
11:40 am	Rice University	Michael Deem
11:50 am	University of California, Berkeley	Martin Head-Gordon, Jeff Neaton, Wendy Queen
12:10 pm	Georgia Tech	David Sholl

Time	Topic	Speaker
12:20 pm	Northwestern University	Randy Snurr
12:30 pm	Advisory Committee	Joachim Sauer
12:40 pm	Working Lunch	
1:30 pm	Guest Presentations	
	1:30-1:40 Ohio State	John Herbert
	1:40-1:50 University of Texas El Paso	Tunna Baruah
	1:50-2:00 Iowa State	Mark Gordon
	2:00-2:10 Cal Tech	Thomas Miller
	2:10-2:20 Stony Brook University	Marivi Fernandez Serra
	2:20-2:30 University of Wisconsin, Madison	JR Schmidt
	2:30-2:40 North Dakota State University	Svetlana Kilina
	2:40-2:50 Pacific Northwest National Laboratory	Bert DeJong
	2:50-3:00 Lawrence Berkeley National Laboratory	Maciej Haranczyk
	3:00-3:10 Oak Ridge National Laboratory	Mark Hagen
3:10 pm	Break	
3:30 pm	Discussion (Moderators: Jeff Long, Joe Hupp, Jeff Neaton, Randy Snurr)	
5:30 pm	Break	
6:00 pm	Dinner	
7:00 pm	Dessert & Presentation on the Institute on the Environment	Lewis Gilbert
7:30 pm	Poster session (conference room C)	
	<ul style="list-style-type: none"> • Peng Bai, et al University of Minnesota • Jose Borreguero, Oak Ridge National Laboratory • Josh Borycz, University of Minnesota • Allison Dzubak & Nora Planas, University of Minnesota • Will Isley, et al. University of Minnesota • Will Isley, David Semrouni, Aaron League, et al, University of Minnesota • Jihan Kim, Lawrence Berkeley National Laboratory • Kyuho Lee, Lawrence Berkeley National Laboratory • Jesse McDaniel, University of Wisconsin, Madison • Jeffrey Sung, Mansi Shah, et al University of Minnesota • Pragya Verma, University of Minnesota • Chun-hung Wang, Washington State University • Federico Zahariev, Iowa State University 	
9:00 pm	End of poster session	
9:10 pm	Shuttle will depart Coffman Memorial Union for Aloft Hotel	

Sunday, November 18, 2012

Campus Club, 4th Floor Coffman Memorial Union, Conference Room A & B

Time	Topic	
8:00 am	Shuttle will depart aloft hotel for Coffman Memorial Union	
8:30 am	Welcome from Director	
8:40 am	Breakout Sessions	Conf Room A&B
	Experiment I (Moderator: Jeff Long)	Conf Room C
	Experiment II (Moderator: Joe Hupp)	
10:30 am	Break	
10:50 am	Breakout Sessions	
	Quantum Methodologies (Moderator: Jeff Neaton)	
	Classical Methodologies (Moderator: Randy Snurr)	
12:30 pm	Working Lunch	
1:30 pm	Group discussion and preparation of final documents	
3:30 pm	Closing Remarks	
3:40 pm	Adjourn	

To arrange your taxi service from the campus club to the airport or the hotel please contact one of the following taxi services to arrange a time that best fits your schedule:

Yellow & White Cab: 612-343-3333

Airport Taxi Mpls: 952-975-9999

Minneapolis West Taxi: 612-275-0000

DOE NANOPOROUS MATERIALS GENOME CENTER
KICK OFF MEETING | UNIVERSITY OF MINNESOTA
POSTER SESSION

Abstracts

Peng Bai,¹ Michael Tsapatsis,¹ and J. Ilja Siepmann^{1,2}

¹Dept. of Chemical Engineering and Materials Science, University of Minnesota

²Dept. of Chemistry, University of Minnesota

Title:

Adsorption of Polar Compounds From Gas and Solution Phases Onto Zeolites

Abstract:

Over the past 20 years, molecular simulation studies have been widely utilized to investigate the adsorption of non-polar and weakly polar species from the gas phase onto zeolites. In contrast, investigations of the adsorption of polar and hydrogen-bonding compounds from a solution phase are very sparse because of a lack of transferable force fields and efficient simulation algorithms for these more complex systems. Here, we present methodological developments that overcome these limitations and apply the new methodologies to adsorptive separations of practical interest. First, the TraPPE-zeo (transferable potentials for phase equilibria-zeolites) force field is parameterized and shown to be capable of predicting the adsorption isotherms for *n*-alkanes, carbon dioxide, alcohols, and water with high accuracy. Second, a simulation strategy is optimized that combines configurational-bias Monte Carlo (CBMC) techniques and the Gibbs ensemble (GE) to allow for the investigation of adsorption from solution phases over the whole composition range (without reliance on empirical activity models) and any number of sorbate species. Third, the TraPPE-zeo force field and CBMC-GE approach are applied to investigate the multi-component adsorption of water, alcohols, and other oxygenated compounds. Silicalite-1 is found to be highly selective for alcohols over water. The ideal adsorbed solution theory substantially underpredicts the amount of sorbed water and leads to very large errors for the sorption selectivity.

Jose M. Borreguero¹, Mark. Hagen¹, Olivier Delaire², Monojoy Goswami³,
Vickie Lynch¹, Andrei Savici¹, Galen Shipman⁴, and Bobby Sumpter^{3,4}

¹Neutron Data Analysis & Visualization Division, Neutron Sciences Directory, Oak Ridge Natl. Lab.

²Materials Science and Technology Division, Physical Sciences Directorate, Oak Ridge Natl. Lab.

³Nanomaterials Theory Institute, Center for Nanophase Materials Science, Oak Ridge Natl. Lab.

⁴Computer Science and Mathematics Division, Computing and Computational Sciences Directorate, Oak Ridge Natl. Lab.

Title:

CAMM Seed Project: Force-Field Refinement by Iterative Fitting to Neutron Scattering Data

Abstract:

The overall aim of the Center for Accelerating Materials Modeling (CAMM) is to develop a software suite that will enable simulation and modeling to be brought directly into the data analysis loop of experimental data taken at the Spallation Neutron Source (SNS). The intent is both to allow the validation of simulations by the experimental data and to allow simulations to predict where new experimental measurements should be performed, and to do this in such a way that it could be implemented in near-real time. The FY13 seed project described here constitutes an initial, core, component of the software toolkit to be developed.

Molecular dynamics (MD) is one of the most commonly used methods for simulating condensed-matter materials. MD force-fields are parameterized from first principles and in some cases refined against available thermodynamics data. Our initial software development in CAMM is a software toolkit to refine MD force-fields against experimental data taken in inelastic, and quasi-elastic, neutron scattering experiments. The structure factors from such experiments are direct probes of the energy spectra (dynamics) of atoms in materials and as such provide a strong test of the accuracy of the MD force-field. The iterative “fitting” engine that we are employing is the DAKOTA package from Sandia National Laboratory which we are configuring for the experimental neutron data and to run the necessary MD simulations. In order to test this process we are initially comparing quasi-elastic neutron scattering data for a concentrated aqueous solution of LiCl to MD-derived (using NAMD) dynamic structure factors. The result of this work has produced a water-model dipole moment that reproduces the dynamics of the experimental ionic solution at standard conditions. The next step in this seed project is to apply this software kit to two more complex cases, from the “soft” and “hard” condensed matter domains respectively, polyethylene oxide (PEO)–acrylic acid (AA) and $\text{KTa}_{1-x}\text{Nb}_x\text{O}_3$, using LAMPPS as the MD package.

Research supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division.

Joshua Borycz

Gagliardi Group, Department of Chemistry, University of Minnesota

Title:

Multi-reference Modeling of Guest-Host Interactions in Open Metal Site Metal-Organic Frameworks

Abstract:

Tunable, adsorbing materials such as Metal-Organic Frameworks (MOFs) are well researched since adsorption within these materials could allow easy capture and transportation of fuels like methane, and might be used to slow the rate of global warming by capturing carbon dioxide. New classes of MOFs that has shown promise for carbon capture have unsaturated metal sites in each unit cell that can selectively adsorb CO₂. The MOF-74 series has been studied experimentally and computationally with various metal centers, but the computational studies have been restricted to single reference (non-resonant) systems. The intermolecular interaction of electron rich, high spin metal centers such as Fe²⁺ with CO₂ may be more accurately modeled by multi-reference methods like Complete Active Space Self-Consistent Field (CASSCF) and Complete Active Space Second-Order Perturbation Theory (CASPT2). A method is proposed that uses CASSCF/CASPT2 to generate the energies of the metal-guest interactions in MOF-74 to generate force field parameters for classical simulation methods such as Grand Canonical Monte Carlo (GCMC).

Allison Dzubak & Nora Planas

Gagliardi Group, Department of Chemistry, University of Minnesota

Title:

Mechanistic study of CO₂ chemisorption in the amine-grafted metal-organic framework mmen-Mg₂(dobpdc).

Abstract:

Much effort has been devoted to the study of CO₂ adsorption within Metal-Organic Frameworks (MOFs) due to their potential use as hosts in industrial gas separation applications. Most of the current studies have focused on understanding physical adsorption of CO₂ to the open metals sites present in these materials, which can be modeled using classical simulation techniques. Here we address the treatment of chemical adsorption in amine-grafted MOFs, where the bond making and breaking between CO₂ and the amine reactive sites must be treated quantum mechanically. We present a mechanistic study for the CO₂-amine reaction with the amine-grafted mmen-Mg₂(dobpdc) using dispersion corrected density functional theory.

William Isley, Cramer, C. J.

The Cramer Group, Department of Chemistry, University of Minnesota

Title:

Benchmarking DFT for Fe(II) Interactions in Small-molecule Models for Fe-MOF-74

Abstract:

We are interested in accurately modeling the chemical behavior and chemi- and physisorption properties of Fe-MOF-74 using computational methods. A first step towards modeling adsorption properties for a periodic material is to select a method which is both accurate and scales favorably with increasing size. The study of the periodic system, or large nanoclusters, with correlated wave function methods would be impractical. In order to facilitate modeling of large systems, we are interested in assessing the suitability of DFT for Fe coordination compounds relevant to the structure of Fe-MOF-74. We describe our benchmarking of DFT models against high level wave function theories and assess accuracy.

William Isley, David Semrouni, Aaron League, Gagliardi, L., Cramer, C. J.
The Cramer Group, Department of Chemistry, University of Minnesota

Title:

Host-Guest Interactions in Metal-Organic Nanomaterials

Abstract:

Host-guest interactions are one way to describe the physics of molecules interacting with the framework of nanomaterials. Here we present a study on the characterization of host-guest interactions for organic molecules encapsulated by a number of self-assembled, metal-templated cages. We quantify and analyze host-guest interactions and the dynamical behavior of the systems using density functional theory and polarizable classical force fields for which we have derived necessary metal parameters. Specific attention will be paid to the special modeling challenges associated with metal-containing nanomaterials.

Jihan Kim¹, Li-Chiang Lin², Mahmoud Abouelnasr², Joseph Swisher^{1,2}, Richard Martin³, Maciej Haranczyk³, Berend Smit^{1,2}

¹Materials Sciences Division, Lawrence Berkeley National Laboratory, ²Department of Chemical and Biomolecular Engineering, University of California, Berkeley.

³Computational Research Division, Lawrence Berkeley National Laboratory

Title:

High-throughput Characterization of Porous Materials for Carbon Capture Applications Using Graphics Processing Unit

Abstract:

We have developed a high-throughput graphics processing units (GPU) code that can characterize and screen a large database of porous materials for carbon dioxide capture. Utilizing the code, the Henry coefficients and self-diffusion coefficients of guest molecules can be computed in few seconds and a complete adsorption isotherm curve can be obtained in few minutes. We present large-scale simulated adsorption and diffusion results for over one hundred thousand pure silica zeolites and aluminosilicate zeolite structures. From this data, we have identified many different structures that have potential to reduce the parasitic energy of carbon capture process by 30-40% compared with near-term technologies. We have also identified free volume and specific configurations of Si/O atoms as key predictors in determining the largest CO₂ uptake for aluminosilicate zeolite structures. Finally, considering membrane applications, we have found many predicted zeolite structures that potentially out-performs the best IZA zeolites by more than five times in CO₂ permeability for CO₂/N₂ and CO₂/CH₄ separations.

Kyuho Lee

Lawrence Berkeley National Laboratory

Title:

Principles and Application of van der Waals Density Functionals

Abstract:

We propose a second version of the van der Waals density functional, denoted as vdW-DF2, of Dion et al., employing an accurate semilocal exchange functional and the use of large-N asymptote gradient correction in determining the vdW kernel. We show that equilibrium separations, hydrogen bond strengths, a van der Waals attractions at intermediate separations longer than equilibria are greatly improved. We also calculate adsorption properties of molecules in metal organic frameworks as application of van der Waals density functionals to extended systems.

Jesse McDaniel

Schmidt Group, Department of Chemistry, University of Wisconsin-Madison

Title:

Computational modeling of gas adsorption in MOFs: Ab initio force field development, efficient lattice model simulations, and exploring the effects of flue-gas contaminants.

Abstract:

Metal organic frameworks (MOFs) are promising materials for use in CO₂ capture/sequestration applications--we employ both quantum mechanical and statistical mechanical computations to study the important properties of MOFs for such applications. Gas adsorption isotherms are of primary interest, and while these are accessible from computer simulations, the accuracy of such calculations is limited by the employed force fields. Due to the numerous reported failures of standard force fields, we have developed ab initio force fields based on symmetry-adapted perturbation theory (SAPT) calculations, and have accurately reproduced CO₂/N₂ experimental isotherms for a variety of zeolitic imidazolate frameworks (ZIFs). These force fields contain distinct terms representing the different types of physical interactions--exchange, electrostatic, induction and dispersion—which not only makes them transferable and robust, but provides valuable insight into the physics determining gas adsorption at different temperatures/pressures. In addition to force field development, we have developed a computationally efficient, lattice model approach for computing gas adsorption isotherms. This lattice model approach allows for orders of magnitude acceleration over conventional grand canonical Monte Carlo (GCMC) methods, enabling high-throughput screening of MOFs for their gas adsorption properties, while employing accurate force fields and lattice sums. For MOFs with coordinatively unsaturated metal sites, in addition to the CO₂/N₂ selectively, the interaction with flue gas contaminants is a concern, as such contaminants have the potential to competitively bind to these open metal sites due to their high adsorption enthalpies. Utilizing primarily density functional theory (DFT) calculations, in addition to Langmuir adsorption models, we have identified potentially problematic contaminant species and have illustrated their possible influence on industrial applications.

Jeffrey Sung,¹ Mansi Shah,² Peng Bai,² and J. Ilja Siepmann^{1,2}

¹Dept. of Chemistry, University of Minnesota

²Dept. of Chemical Engineering and Materials Science, University of Minnesota

Title:

Simulating Complex Chemical Systems

Abstract:

The Siepmann group develops efficient sampling algorithms and accurate force fields and applies these to investigate complex chemical systems and processes including microheterogeneous fluids, green solvents, chromatographic separations, phase and sorption equilibria, atmospheric nucleation and Earth materials. This poster provides information on the Siepmann group's research expertise to stimulate collaborative projects with other NMG Center researchers.

Pragya Verma

Truhlar Group, Department of Chemistry, University of Minnesota

Title:

Modeling Metal-Organic Frameworks for Paraffin/Olefin Separation

Abstract:

Separation of paraffin/olefin mixtures has several important commercial applications and hence, devising cost-effective and environment-friendly gas separation procedures is highly required. Current methods of separation, such as cryogenic distillation, manifest considerable technical and economic barriers. Metal-organic frameworks (MOFs), which are sponge-like crystalline nanoporous materials with exceptionally high porosity and surface areas, provide cost-effective alternates to separation at higher temperatures, dispensing the need for cryogenic cooling, thus making them promising materials for future research in separation. An iron-based MOF, Fe-MOF-74, is particularly useful for the fractionation of paraffin/olefin mixtures.¹ Computational approaches can be useful in obtaining a wealth of information about the binding sites, interaction energies, isosteric heats, isotherms, separation factors and other properties of adsorption, complementing experimental data. To gain insight into the structure and binding properties of Fe-MOF-74, we are studying three model systems representative of the MOF: one-, three-, and five-iron models with increasing levels of resemblance to the X-ray crystal structure, and investigating their binding to ethane and ethene. The one-iron model, FeF₂, is a test model, whose binding to ethane and ethene has been studied using various members of the Minnesota family of density functionals, such as M05, M06, M06-L, M11-L, MN12-L, and MN12-SX, as well as SOGGA11, SOGGA11-X, and N12-SX. The three- and five-iron models are 88- and 106-atom model systems, respectively, carved out of the X-ray crystal structure of Fe-MOF-74. Most calculations on the three- and five-iron models were carried out with M06-L.

[1] Bloch, E. D.; Queen, W. L.; Krishna, R.; Zadrozny, J. M.; Brown, C. M.; Long, J. R. *Science* **2012**, 335, 1606.

Chun-Hung Wang

The A. Clark Group, Department of Chemistry, Washington State University

Title:

Graph Theory Applications in Chemical Dynamics and Structural Data Mining

Abstract:

Graph theory investigates the connection and dynamic changes in a graph over time. Any network of object interacting with one another can be turned into a graph, therefore graph theory has been applied in various chemical dynamic systems and structural data mining. The link analysis algorithm PageRank has been widely used in weighing the hyperlinked set such as Google search. Combined with the chemical constraints of a system, PageRank can be used to identify the polyhedral arrangements of H-bonding in water system. Applied in metal-organic framework (MOF) system, the hyperlink between methane and MOF to study intermolecular interactions for methane storage can be investigated.

Federico Zahariev^a, L. Roskop^b, and M. S. Gordon^c
Mark Gordon Research Group, Ames Laboratory, Iowa State University

Title:

Water-silica interactions by fragmentation methods

Abstract:

The interaction of water with silica has two aspects. First, the ideal silica structure has a very low reactivity towards water. Nevertheless the geometrical constraints of silica pores as well as the water-silica interactions affect the structure of water. As a preliminary step towards the investigation of the diffusion of water in mesoporous silica a tubular silica model is constructed and the energy profile of a single water molecule passing through the model silica pore is computed by the Fragment Molecular Orbital (FMO) method. Second, defects on the surface of silica act as reaction centers for surface hydrolysis. Aspects of water-silica surface reactions are investigated by the Integrated Molecular Orbital/Molecular Mechanics optimization scheme for Surfaces (SIMOMM) method.

a) federico@si.msg.chem.iastate.edu

b) luke@si.msg.chem.iastate.edu

c) mark@si.msg.chem.iastate.edu

Nanoporous Materials Genome Center Kick Off Meeting

November 17-18, 2012 | University of Minnesota

Participants

Peng Bai	University of Minnesota
Tunna Baruah	University of Texas, El Paso
Jose Borreguero	Oak Ridge National Laboratory
Josh Borycz	University of Minnesota
Rebecca Carlson	University of Minnesota
Aurora Clark	Washington State University
Chris Cramer	University of Minnesota
Michael Deem	Rice University
Bert DeJong	Pacific Northwest Nat'l Laboratory
Allison Dzubak	University of Minnesota
Marivi Fernandez Serra	Stony Brook University
Laura Gagliardi	University of Minnesota
Danell Garber	University of Minnesota
Mark Gordon	Iowa State University
Mark Hagen	Oak Ridge National Laboratory
Maciej Haranczyk	Lawrence Berkeley National Laboratory
Martin Head-Gordon	University of California, Berkeley
John Herbert	The Ohio State University
Chad Hoyer	University of Minnesota
Joseph Hupp	Northwestern University
Will Isley	University of Minnesota
Svetlana Kilina	North Dakota State University
Jihan Kim	Lawrence Berkeley National Laboratory
Aaron League	University of Minnesota
Kyuhoo Lee	Lawrence Berkeley National Laboratory
Jeff Long	University of California, Berkeley
Ben Lynch	Univ. of Minnesota- Supercomputing Inst.
Rémi Maurice	University of Minnesota
Jesse McDaniel	University of Wisconsin, Madison

Nanoporous Materials Genome Center Kick Off Meeting

November 17-18, 2012 | University of Minnesota

Participants

Thomas Miller	Cal Tech
Jeff Neaton	Lawrence Berkeley National Laboratory
Mark Pederson	U.S. Department of Energy
Nora Planas	University of Minnesota
Wendy Queen on behalf of Omar Yaghi	Lawrence Berkeley National Laboratory
Joachim Sauer	Humboldt University, Berlin, Germany
JR Schmidt	University of Wisconsin, Madison
David Semrouni	University of Minnesota
Mansi Shah	University of Minnesota
Huiliang Shi	University of Minnesota
David Sholl	Georgia Tech
Ilja Siepmann	University of Minnesota
Berend Smit	University of California, Berkeley
Randy Snurr	Northwestern University
Jeffrey Sung	University of Minnesota
Don Truhlar	University of Minnesota
Michael Tsapatsis	University of Minnesota
Pragya Verma	University of Minnesota
Chun-hung Wang	Washington State University
Federico Zahariev	Iowa State University