Workshop on Atomistic Simulations for Industrial Needs
Theme: Computational, Simulation, and Experimental Investigation of Materials for Gas Separations
July 22-23, 2014

National Institute of Standards and Technology, Gaithersburg, Maryland
NIST Administration Building (101), Lecture Room B
Organizers: Chandler Becker, Fred Phelan, and Dan Siderius (NIST)

Tuesday, July 22

9:00 AM	Welcome and Introductions	Becker, Phelan, Siderius
9:30 AM	Designing structured carbon sorbents for CO2 capture through experimental and Monte Carlo simulation insights	Erik Rupp; Stanford
10:00 AM	Modeling the adsorption-induced breathing of nanoporous carbon	Carlos Wexler; U. Missouri
10:30 AM	Adsorption in flexible structures: experiment and modeling	Peter Ravikovitch; ExxonMobil Research
11:00 AM	*Break*	
11:30 AM	Towards metal-organic framework adsorbents and membranes for gas separations: A combined computational-experimental approach	Sankar Nair; Georgia Tech
12:00 PM	Discussion	
12:30 PM	*Lunch (NIST cafeteria)*	
1:30 PM	Posters	
2:00 PM	Ab initio modeling of adsorption and reaction of CO2 and H2 in Lewis Pair functionalized metal organic frameworks	J. Karl Johnson; U. Pittsburgh
2:30 PM	Carbon capture properties of nanoporous solid materials	Lan Li; Boise State
3:00 PM	Development of a piezoelectric molecular dynamics model for boron nitride nanotubes	Vesselin Yamakov; NASA
3:30 PM	*Break*	
4:00 PM	Discussion: What are the outstanding needs for designing these materials?	
5:00 PM	*Adjourn for day*	
6:30 PM	*Dinner, That's Amore*	

Wednesday, July 23

9:00 AM	Large-scale screening for adsorption behavior of complex molecules in zeolites	Ilja Siepmann; U. Minnesota
9:30 AM	High-throughput computational screening of metal-organic frameworks for gas separation applications	Randall Snurr; Northwestern
10:00 AM	Usability and Reproducibility: Proper Programming Practices in Science	Patrick Fuller; NuMat
10:30 AM	*Break*	
11:00 AM	Interrogating Simple Pore Models using Flat-Histogram Sampling Methods to Understand the Effect of Adsorbent Flexibility on Fluid Adsorption	Daniel Siderius, Vincent Shen; NIST
11:30 AM	NIST Measurement Capabilities for Gas Sorption and Porous Materials Characterization	Laura Espinal; NIST
12:00 PM	*Discussion (wrap-up)*	
12:30 PM	*Lunch (NIST Cafeteria)*	
1:30 PM	Demonstrations and Tutorials	
	WebFF, a force field repository for soft materials	Huai Sun
	DSpace for archiving data and supporting information	Chandler Becker
	Simulation automation and reproducibility with Python	Zachary Trautt
	NIST/ARPA-E Database of Novel and Emerging Adsorbent Materials	Daniel Siderius
2:30 PM	Tours of the *Facility for Adsorbent Characterization and Testing*	Laura Espinal; NIST
3:00 PM	*Adjourn Workshop*	