

CoMSEF Newsletter

AIChE[®]

CoMSEF General Meeting in Pittsburgh

CoMSEF will hold its annual General Meeting on Wednesday October 31 from 6:15-7:15 p.m. in 412 (convention center) during the Fall 2012 AIChE Meeting. As in the past, the meeting will be held jointly with Area 1a (Thermodynamics and Transport Properties). All CoMSEF members are encouraged to attend. The winners of the CoMSEF Graduate Student Awards will be announced, and Fernando Escobedo will be presented with the 2012 Impact Award.

CoMSEF Elections

The annual CoMSEF election is currently underway. This year we will elect a vice-chair, secretary/treasurer, and two Liaison Directors. Information about the candidates and the duties of each office can be found at <http://comsef.org/election-2012>. You should have received voting instructions by email. If you didn't receive the email or lost it, contact admin@comsef.org for help. The deadline for casting your vote is October 22th.

October 2012

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Fernando Escobedo 2012 CoMSEF Impact Award Winner



Professor Fernando Escobedo of Cornell University has been selected as the recipient of the 2012 CoMSEF Impact Award. This annual award recognizes outstanding research in computational molecular science and engineering and will be given to Fernando during the CoMSEF General Meeting at the AIChE Annual meeting in Pittsburgh. He will also present a talk on his research at the CoMSEF Plenary Session at the AIChE Annual meeting.

Fernando is the Marjorie Hart Chair of Chemical Engineering at Cornell. He received his Bachelor's degree in Chemical Engineering at Universidad de San Augustin, Peru, a Master's degree in Chemical Engineering from the University of Nebraska-Lincoln, and a PhD in Chemical Engineering from the University of Wisconsin-Madison.

Fernando has made important contributions to the development of new computational methods, which he has then applied to the solution of important problems in the area of complex fluids, including polymers, colloids, and peptides. He is receiving the CoMSEF Impact Award "*For the elucidation and prediction of complex phases formed by block copolymers, elastomers, and polyhedral particles, and the advancement of novel Monte Carlo simulation methods*". CoMSEF Impact Award recipients must be within 15 years of completion of their highest degree and be current members of CoMSEF.

2012 CoMSEF Graduate Student Awards

The CoMSEF Graduate Student Awards in Computational Molecular Science and Engineering will be awarded for the 8th consecutive year at the annual AIChE Meeting in Pittsburgh. The awards recognize excellence in research by graduate students in the field of computational molecular science and engineering. Two awardees will be selected based on the nomination letters received from each students' advisor and a poster presented at the CoMSEF poster session (session #178) to be held Monday evening from 6 - 8 pm. The winners will be announced at the CoMSEF/Area 1a annual General Meeting (Wednesday, from 6:15-7:15 pm, 412 in the convention center).

Renew Your Membership and Get a Friend to Join!!

It's renewal time!!! CoMSEF membership is a great way to promote activities and sessions in computational molecular science at the Annual AIChE Meeting. As a CoMSEF member, you will receive an electronic copy of our semi-annual newsletter (which highlights CoMSEF activities, members, opportunities, and recent papers in the literature) and occasional postings about job openings/upcoming conferences. Your membership dues support CoMSEF awards that garner recognition for outstanding graduate students and faculty in computational molecular science and engineering. As a CoMSEF member, you can be nominated (if eligible) for one of the CoMSEF awards. Convince a student or colleague to join! Student membership is FREE!! To renew your CoMSEF membership for another year, go to: <http://www.iche.org/community/divisions-forums>

The 7th Industrial Fluid Properties Simulation Challenge

Zeolite adsorbents are used in a variety of applications due to their high surface area and ability to adsorb or desorb sorbates depending upon the applied conditions. Applications include the removal of volatile organic compounds and toxic gases from air and storage of corrosive chemicals during shipping. With increasing numbers of applications, the ability to predict the performance of zeolites for a wide range of adsorbents would be very valuable in pre-optimizing systems and reducing product development time. Molecular simulation techniques, in principle, could be ideal for predicting adsorption in zeolites with various chemistry. The focus of the current challenge is to assess the potential of molecular simulation methods to predict organic sorbate adsorption isotherms. Specifically, the challenge will focus on predicting the adsorption isotherms of n-perfluorohexane in BCR-704 Faujasite type zeolite. More info is here: <http://fluidproperties.org/>

Five entries for the challenge have been received. At session #775 (Thursday, November 1, 2012: 3:15 PM, 415, Convention Center) the benchmark data will be discussed, the entrants will present their work, and the champions will be announced. Information about the next challenge (8th) will also be discussed. Please join us!

Annual Meeting Sessions

CoMSEF has an exciting range of programming on offer at the upcoming 2012 AIChE Annual Meeting in Pittsburgh, with over 30 sponsored and co-sponsored sessions. Of special note are the Computational Molecular Science and Engineering Forum Plenary Session at 12:30 on Wednesday and the CoMSEF Poster Session on Monday from 6:00-8:00 pm. There are also two sets of sessions honoring two celebrated members of our community. A pair of sessions in honor of Keith Gubbins' 75th birthday begins on Monday morning at 8:30 am, and a series of sessions honoring Alexis Bell's 70th birthday begin on Tuesday at 8:30 am. Full details on all of the CoMSEF sessions are available at: <http://aiche.confex.com/aiche/2012/webprogram/21.html>

Upcoming Conferences of Interest to CoMSEF Members

APS March Meeting 2013

March 18 - 22, 2013
Baltimore, MD
<http://www.aps.org/meetings/march/index.cfm>

ACS National Meeting and Exposition Spring 2013

April 7 - 11, 2013
New Orleans, LA
<http://portal.acs.org/>

2013 MRS Spring Meeting

April 1-5, 2013
San Francisco, CA
<http://www.mrs.org/spring2013/>

PPEPPD 2013

May 26-30, 2013
Iguazu Falls, Argentina - Brazil
<http://www.ppeppd2013.plapiqui.edu.ar/openconf.php>

27th IEEE International Parallel & Distributed Processing Symposium

May 20-24, 2013
Hyatt Regency Cambridge, Boston, Massachusetts
<http://www.ipdps.org/>

STATPHYS25 — XXV IUPAP International Conference on Statistical Physics

22 Jul 2013 - 26 Jul 2013
Seoul, South Korea
<http://www.statphys25.org>

VII BRAZILIAN MEETING ON SIMULATIONAL PHYSICS

6th Aug 2013 - 10th Aug 2013
Joao Pessoa, Brazil
<http://www.fisica.ufpb.br/bmisp/>

Thermodynamics 2013

03 Sep 2013 - 06 Sep 2013
Manchester, United Kingdom
<http://www.thermodynamics2013.org/>

Materials for a Sustainable Energy Future
September 9 – December 13, 2013
Institute for Pure and Applied Math, UCLA, Los Angeles, CA
<http://www.ipam.ucla.edu/programs/mse2013/>

Research Highlight: Current State of Molecular Dynamics Simulations on Graphics Processing Units (GPUs)

by Arthi Jayaraman

Recent progress in graphics processing units (GPUs) and simultaneous development of molecular simulation algorithms designed for or adapted to run optimally on GPUs have enabled molecular modelers to dream of “larger” and “longer” simulations than they have done so far. This “coming of age” of GPUs in the field of molecular simulations has been covered in a recent review by Stone et al. in 2010 [1]. The release of both CUDA, a GPU programming toolkit that enables parallel execution of functions called ‘kernel’ on NVIDIA GPUs, and OpenCL, a multi-platform data-parallel programming interface for computing on GPUs, have enabled molecular dynamics (MD) packages to incorporate GPU acceleration. What makes MD simulations of macromolecules perfect for implementation on GPUs is their computational complexity and parallelism. While packages that were originally designed for parallel central processing units (CPUs) implementation, like NAMD [2] and LAMMPS [3] have now incorporated GPU compatibility, there are other new packages like HOOMD-blue [4] that have explicitly been designed for GPU execution. With these developments, one is able to achieve order(s) of magnitude speedups compared to the same simulations on CPUs in a variety of coarse-grained particle simulations that would have been impractical without access to enormous computational resources. Stone et al. [1] cite, for example, a recent study by Glotzer and co workers [5], aimed at studying stability of the double gyroid phase in a soft materials system which required more than 600 different simulation runs of 48 GPU-hours apiece; with LAMMPS the same study would have needed ~ 1 million CPU-hours. In addition to obtaining MD trajectories, data analysis of trajectories involving histograms also perform well on GPUs due to their intrinsic parallelism. For example, a recent paper [6] shows how radial distribution function histogramming can be implemented on multiple NVIDIA GPUs allowing cumbersome data analysis on large trajectories to be conducted in seconds-few minutes. In addition to these papers highlighting the successes of these simulation and analysis methods on GPUs, the simulations community is also focusing on potential implications of the choice of the (single/double) precision model with GPU implementation [4,7,8]. For example, recent work by Gotz et al [7] shows that in case of MD simulations of biomacromolecules with implicit solvent using AMBER on GPUs, “the numerical noise due to rounding errors within the single precision model was sufficiently large to lead to an accumulation of errors which can result in unphysical trajectories for long time scale simulations.” They have gone on to develop “a hybrid precision model for floating point arithmetic that provides performance close to full single-precision calculations but retains energy drifts in constant energy MD simulations and structural properties of proteins for long time scale MD simulations equivalent to what is achievable with full double precision.” Concurrently other studies, for example one by Taufer et al.[8], have been conducted to show that these energy drifts can be substantially reduced, while maintaining high performance similar to single precision GPUs, by making use of a “new numeric type composed of multiple single precision floating-point numbers”, thus improving numerical reproducibility and stability of large-scale parallel MD simulations on GPUs. The above development and evaluations of reproducibility and stability of GPU based computations continue to transform the field of molecular simulations, allowing scientists to revisit simulations of problems that were intractable in the past with CPUs alone.

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- [2] www.ks.uiuc.edu/Research/namd/ Scalable molecular dynamics with NAMD J.C. Phillips, R. Braun,W. Wang, J. Gumbart, E. Tajkhorshid, E. Villa, C. Chipot, R.D.Skeel, L. Kale, K. Schulten, J. Comp. Chem. 26 (2005) 1781–1802. <http://10.1002/jcc.20289>
- [3] <http://lammms.sandia.gov> and Fast parallel algorithms for short-range molecular dynamics, S.J. Plimpton, J. Comp. Phys. 117 (1995) 1–19. <http://dx.doi.org/10.1006/jcph.1995.1039>
- [4] <http://codeblue.umich.edu/hoomd-blue> Molecular Dynamics on Graphic Processing Units: HOOMD to the Rescue. Joshua A. Anderson and Alex Traveset Computing in Science & Engineering 10(6) (2008). General purpose molecular dynamics simulations fully implemented on graphics processing units Joshua A. Anderson, Chris D. Lorenz, and Alex Traveset, Journal of Computational Physics 227 (2008) 5342-5359. <http://dx.doi.org/10.1016/j.jcp.2008.01.047>
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- [7] Routine Microsecond Molecular Dynamics Simulations with AMBER on GPUs. 1. Generalized Born Andreas W. Götz Mark J. Williamson, Dong Xu, Duncan Poole, Scott Le Grand, and Ross C. Walker J Chem Theory Comput. 2012; 8(5): 1542–1555. <http://dx.doi.org/10.1021/ct200909j>
- [8]: Improving numerical reproducibility and stability in large-scale numerical simulations on GPUs. Michela Taufer, Omar Padron, Philip Saponaro, Sandeep Patel, IPDPS 2010: 1-9

Research Highlight: Density functional theory with screened van der Waals interactions

By Cynthia Lo

Organic-based interfaces possess electronic properties that are increasingly being explored for use in emerging devices, such as (opto)-electronics, organic photovoltaics, and sensors. Modeling the structure and properties of these hybrid inorganic-organic systems requires knowledge of how organic molecules, such as benzene or 3,4,9,10-perylenetetracarboxylic acid dianhydride (PTCDA), adsorb to transition metal surfaces. In particular, the accurate treatment of covalent interactions, electron transfer processes, van der Waals (vdW) interactions, and Pauli repulsion is a challenging problem for density functional theory calculations (DFT). In recent years, much attention has been focused on accurate modeling of vdW interactions, since the local density approximation (LDA) to DFT underestimates binding distances and the generalized gradient approximation (GGA) predicts a zero energy of binding for PTCDA on Ag(111). The popular interatomic pair-wise PBE-D correction [1] correctly predicts the experimental binding distance, but overestimates the binding energy by 1 eV. The recently introduced DFT + vdW^{surf} correction scheme calculates the vdW C6 coefficients and radii nonempirically from the electron density [2], and incorporates the Lifshitz-Zaremba-Kohn (LZK) theory [3,4] that includes the many-body collective response (screening) of the substrate electrons; essentially, by going effectively beyond the pairwise description, vast improvements in both binding distance and binding energy are observed when compared to all other theoretical methods.

In the recent work by Ruiz et al. [5] and the follow-up by Liu et al. [6], the authors use DFT + vdW^{surf} to model PTCDA and benzene adsorption to the (111) surfaces of Cu, Ag, Au, Pt, Pd, Rh, and Ir. This method successfully reproduces the vertical distortion experienced by the PTCDA molecule upon adsorption on Ag(111) and Cu(111). By analyzing the strength of benzene adsorption to these metal surfaces, the authors also determined that there is a significant concerted effect of covalent bonding and vdW interactions for benzene interacting with metal surfaces, which leads to qualitative changes in the adsorption behavior when vdW interactions are accurately included and treated. Thus, vdW forces contribute significantly to the stabilization of strongly adsorbed benzene on (111) surfaces of Pt, Pd, Rh, and Ir metals, as compared to physisorption on the (111) surfaces of Ag and Au. Much of this effect is attributable to the partially empty *d*-band of the Pt, Pd, Rh, and Ir, compared to the fully occupied *d*-band of Au and Ag. In Pt, for instance, Pauli repulsion is weakened by the rearrangement of *d*-electron density as the benzene molecule approaches the Pt surface, and the HOMO and LUMO levels of the combined system broaden and hybridize noticeably. This vdW-induced behavior (i.e., broadening, shift, hybridization of levels, and electron transfer) may account for the enhanced electronic properties of these hybrid inorganic-organic systems. Furthermore, the DFT + vdW^{surf} method has the same computational cost as the underlying DFT calculation* and is equally applicable to insulators, semiconductors, and metals.

[1] S. Grimme, J. Comput. Chem. 27, 1787 (2006). <http://dx.doi.org/10.1002/jcc.20495>

[2] A. Tkatchenko and M. Scheffer, Phys. Rev. Lett. 102, 073005 (2009). <http://dx.doi.org/10.1103/PhysRevLett.102.073005>

[3] E. M. Lifshitz, Sov. Phys. JETP 2, 73 (1956).

[4] E. Zaremba and W. Kohn, Phys. Rev. B 13, 2270 (1976). <http://dx.doi.org/10.1103/PhysRevB.13.2270>

[5] V. G. Ruiz, W. Liu, E. Zojer, M. Scheffer, and A. Tkatchenko, Phys. Rev. Lett. 108, 146103 (2012). <http://dx.doi.org/10.1103/PhysRevLett.108.146103>

[6] W. Liu, J. Carrasco, B. Santra, A. Michaelides, M. Scheffler, and A. Tkatchenko, <http://arxiv.org/abs/1209.4345>

* However, if structural optimization is performed, this method is much more expensive than the underlying DFT.

Member Spotlights

The "member spotlight" is a new newsletter feature intended to introduce CoMSEF members (selected at random) to the rest of the CoMSEF membership.



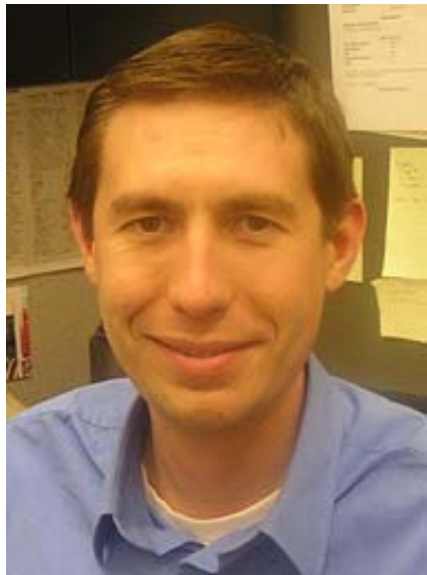
Mike Janik (Penn State University)

I am an Associate Professor of Chemical Engineering at Penn State and hold the John and Jean Brennan Clean Energy Chair. After receiving my B.S. in Chemical Engineering from Yale University, I worked as a Process Engineer for Procter and Gamble. I returned to graduate school at the University of Virginia and completed my Ph.D. under the joint guidance of Matt Neurock and Bob Davis. In 2006, I joined the faculty at Penn State. Our research uses computational techniques, mainly first-principles methods, to examine materials challenges in catalysis and other energy technologies.

As an engineer motivated to make a difference in energy and environmental technology, I have been drawn to the field of catalysis since my undergraduate studies. I began graduate school having no tangible picture of what it meant to pursue computational research. After joining a collaborative experimental/computational project, my fascination with quantum mechanics, interest in programming and numerical methods, and tendency to break glassware officially turned me to the (in the words of Bob Davis) "dark side." My desire to

make a difference in practical technologies has remained, and I enjoy now teaching student researchers how to apply computational chemistry tools to advance applications in energy technology. <http://www.che.psu.edu/Faculty/Janik/>

Daniel Siderius (National Institute of Standards and Technology)



I am a research chemical engineer at the National Institute of Standards and Technology (NIST) in Gaithersburg, Maryland, where I work with the Chemical Informatics Group in the Material Measurement Laboratory. My work at NIST has two intertwining focuses: The first is computational research using molecular simulation and other tools to investigate phase behavior of confined fluids (mainly for applications in gas adsorption), aggregation behavior of proteins, and structural characterization of sorbent materials. The second is the generation and collection of high quality simulation data describing material and fluid properties, similar to standard reference materials or standard reference data; our goal is to generate very reliable simulation data that can be used for algorithm development, as reference data, or in original research by end-users outside NIST. The "NIST Standard Reference Simulation Website" is the main vehicle that we use to disseminate this data at present http://www.nist.gov/mml/csd/informatics_research/srsw.cfm. I find this work very enjoyable and satisfying, particularly since it lies at the intersection of several fields that have fascinated me for years (chemistry, physics, and mathematics).

It could be said that my interest in computational molecular science began as a sort of misunderstanding while I was searching for a graduate program. When I was studying for my B.S. in Chemical Engineering at Michigan Technological University, I became very interested in chemical process simulation and the associated thermodynamics of phase equilibria, so I naturally gravitated toward graduate programs that listed "computer simulation" in their

research portfolio. While speaking with David Corti about his research group and open projects, I quickly realized that "computer simulation" meant "molecular simulation" in his case. Nonetheless, I found his research tools and applications very interesting and worked for Prof. Corti while completing the M.S. and Ph.D. programs in Chemical Engineering at Purdue University. Afterward, I spent two years as a post-doc with Lev Gelb at Washington University in St Louis and then an additional two years at NIST as an NRC Research Associate before being converted into a regular staff scientist.

Patrick Warren receives Ig Nobel honor for “ponytail physics”

Patrick Warren (for example, of DPD fame <http://dx.doi.org/10.1063/1.474784>) and colleagues received an “Ig Nobel” award at a recent ceremony held at Harvard University. Their “Ponytail Shape Equation” and “Rapunzel Number” enable shape predictions for hair that is pulled together and bound behind the head. The work was documented in an article in Physical Review Letters (<http://dx.doi.org/10.1103/PhysRevLett.108.078101>). More info about Warren and the award can be found in the BBC News report (<http://www.bbc.co.uk/news/science-environment-19667664>) and at the Ig Nobel web site (<http://www.improbable.com/ig/>). Congratulations to Patrick!