Computational Molecular Science and Engineering Forum
for the combined community of engineers and scientists developing and applying molecularly based theories, modeling, and simulation
http://comsef.org/

CoMSEF Newsletter

AIChE

October 2019

In This Issue

Peters Winner of 2019 CoMSEF Impact Award

Professor Baron Peters from the Departments of Chemical Engineering and Chemistry and Biochemistry at the University of Illinois is the winner of the 2019 CoMSEF Impact Award. He is cited for "***simulation techniques using special "rare events" that deepen understanding of crystal nucleation and growth, catalysis by amorphous materials, and of reactions in polar solvents***." Prior to joining the faculty at Illinois in 2019, Baron was most recently a professor of chemical engineering at the University of California, Santa Barbara (UCSB). Peters received his PhD from the University of California, Berkeley, in 2004. For his post-doctoral research, he worked with Bernhardt Trout at the Massachusetts Institute of Technology and with Berend Smit at the Centre Européen de Calcul Atomique et Moléculaire. Peters was on the chemical engineering faculty at UCSB from 2007 to 2018. Baron will receive his award during the CoMSEF Plenary Session at the 2019 AIChE Annual Meeting, where he will also deliver a presentation describing his research. The CoMSEF Impact Award is given annually to a CoMSEF member who is within 15 years of completion of their highest degree.

Haji-Akbari Winner of the 2019 CoMSEF Young Investigator Award

Professor Amir Haji-Akbari from the Department of Chemical Engineering at Yale University is the 2019 winner of the CoMSEF Young Investigator Award. He is cited for "***his pioneering contributions to developing and utilizing advanced sampling techniques to study crystallization, including colloidal self-assembly and ice nucleation***." Prior to joining the faculty at Yale in 2017, Amir was a Postdoctoral Research Associate at Princeton University in Pablo Debenedetti's group. Amir received his PhD in chemical engineering from the University of Michigan in Ann Arbor in 2011. Amir will receive his award during the CoMSEF Plenary Session at the 2019 AIChE Annual Meeting, where he will also deliver a presentation describing his research. The CoMSEF Young Investigator Award is given annually to a CoMSEF member who is within 7 years of completion of their highest degree.

2019 CoMSEF Graduate Student Awards

The CoMSEF Graduate Student Awards in Computational Molecular Science and Engineering will be awarded at the annual AIChE Meeting in Orlando. The awards recognize excellence in research by graduate students in the field of computational molecular science and engineering. The awardees will be selected based on the nomination letters received from each student's advisor, their CV, and a poster presented during the CoMSEF poster session, which will be held Tuesday afternoon from 3:30 to 5:00 PM in Hyatt Regency Orlando - Regency Ballroom R/S. The winners will be announced at the CoMSEF/Area 1a General Meeting (Wednesday, from 6:15-7:15 pm).

CoMSEF General Meeting in Orlando

CoMSEF will hold its annual General Meeting on Wednesday November 13 from 6:15-7:15 pm in Hyatt Regency Orlando - Rock Spring I/II. 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 and the Liaison Directors election results will be announced. Programming for future AIChE meetings will also be discussed.

CoMSEF Elections

The annual CoMSEF election is currently underway. This year we will elect Liaison Directors and vote on two proposed changes to the by-laws. Information about the candidates, the duties of the office, and the proposed by-law changes can be found at http://comsef.org/elections-2019. 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 Monday October 28th.

A Broader View: Supporting and Advocating for your Postdocs

Clare McCabe, Chemical and Biological Engineering, Vanderbilt

Let's start by being sure we are all on the same page. What is a postdoc? According to the National Postdoc Association, a postdoc is "*[an] individual who has received a doctoral degree (or equivalent) and is engaged in a temporary and defined period of mentored advanced training to enhance the professional skills and research independence needed to pursue his or her chosen career path."* Note the words temporary and mentored. We all know that a postdoc is an extended period of training beyond the PhD; but when does temporary become permanent? In 2014, the National Academies recommended a 5-year limit to postdoc training and it's gained a lot of traction, with many schools now capping the training period and encouraging more appropriate research faculty and staff positions for those people with >5 years of experience. The other important keyword is mentoring, which is where we, as PIs, really can have an impact at the individual level. Do you help your postdocs get the skills they need to succeed beyond your lab? Do you allow them time to pursue the professional development activities they need to figure out what their next steps should be and what skills they need? We all should. Whether they want to follow you into academia or see an industrial position in their future we all need to know how to teach, how to lead, and how to have critical conversations. And doesn't having someone with those skills in your lab ultimately also help you and your research group? Research has shown that graduate students that teach are more productive for example; investing in your postdocs is worth it!

Postdocs are often the forgotten group on campus – central to the research mission yet mostly invisible and plagued by feelings of isolation. In an effort to address the needs of this important population in the last 5+ years, several schools have established postdoc offices to provide a focal point for *all-things* postdoc. In this authors' opinion, as a director of a postdoc office and so in the interest of full disclosure obviously biased, a postdoc office is essential to provide support and guidance to the postdocs and the faculty that mentor them (and staff that process all the pesky administrative stuff). A postdoc office can ensure an institution is following recommendations for best practices from the National Postdoc Association and the National Academies. These recommendations cover the five main aspects of the postdoctoral experience: period of service, title and role, career development, compensation and benefits, and mentoring.

While we as PIs cannot change institutional policies overnight, we can advocate for change and at least make the life of the postdocs in our own labs better. We can make sure that we mentor our postdocs to position them for the career they aspire to, we can make sure we do not keep scholars in long term postdoc positions when they should be transitioned to other higher paying positions. If your institution does not mandate a minimum pay for postdocs based on years of experience, make sure you follow the NIH postdoc stipend chart for salary and pay an appropriate salary based on years of experience and encourage your colleagues to do the same. Allow your postdocs time away from the lab and have a clear leave policy so they feel at ease asking for time away. We all do our best work when we have adequate time to tend to our needs outside of the workplace; I encourage you to empower your postdocs to take breaks as needed (as a point of reference, the current NIH guideline is 22 days a year). Encourage your postdocs to complete an individual development plan and think about their short - and long-term goals – when they know where they are going it is easier to plan and help them develop the skills they need. Help your postdocs network and make the connections they need!

Slowly the attitudes towards and understanding of postdocs' concerns is changing, but we can all do our bit by speaking up and looking out for those postdocs that we do have the pleasure of interacting with.

Research Highlight: Extending the Reach of Atomistic Simulations Through Machine-Learned Reactive Interatomic Potentials

Rebecca K. Lindsey, Physical and Life Sciences Directorate, Materials Science Division, Lawrence Livermore National Laboratory

It can be stated with no uncertainty that computers are an integral component of modern-day research, enabling automation, simulation, and data processing. Over the past century, atomistic simulations have progressed from 2D systems of 224 hard disks to those containing 10^{12} atoms and have been applied to countless chemical problems. Though this relentless progress is most typically attributed to Moore's Law, impact of the underlying interatomic interaction potentials (IIPs) should not be overlooked.

Ideally IIPs would afford the accuracy of first principles methods at the expense of a molecular mechanics model. As it stands, a manifold of models leveraging low-complexity, high-efficiency descriptions for interatomic interactions (e.g. Lennard-Jones, Mie, Buckingham, square-well, etc.) is available for problems spanning drug delivery in biological systems to separations for industrial research. However, there are relatively few models capable of accurately describing *chemistry* in organic molecular materials (notable examples including: ReaxFF, REBO, and GAP). Developing parameter sets for these oft convoluted models is an onerous task; one must carefully consider physical suitability of the numerous underlying model equations, generate large volumes of first-principles-derived training data, and ultimately, optimize 10s to 100s of non-linear parameters in such a

manner that the resulting potential energy surface remains smooth. With these considerations in mind, the relative scarcity of reactive IIPs for organic molecular systems is unsurprising.

In recent years, machine learning (ML) has gained significant traction among the model development community due to its versatility and potential to considerably decrease the human effort required to generate high-fidelity models for complicated systems. The potential benefits of ML-IIP development are three-fold: (1) facile parametrization of high-dimensionality problems, (2) a "learned" rather than assumed relationship between system structure and potential energy, (3) automated training repository construction.

The recently developed ANI[1–4] family of actively-learned neural network potentials provide a compelling case for the viability of ML-IIPs. In particular, these models have been shown capable of coupled-clusters accuracy for conformational energetics and thermochemistry, are generally transferable across C, H, O, and N-containing species, and are *billions* of times more efficient than the reference quantum mechanical method. ANI IIPs also hold promise as an alternative route to training data for development of *other* IIPs, particularly in cases where first principles-derived forces and/or energetics are sought for species who size that would be otherwise prohibitive. Moreover, systematic improvements to the ANI methodology have provided insights on practical application of many ML approaches to the chemical sciences. Ultimately, this work brings the field closer to bridging the gap between first principles and molecular mechanics simulation approaches.

[1] Smith, J. S., Isayev, O. & Roitberg, A. E. ANI-1: "An extensible neural network potential with DFT accuracy at force field computational cost" *Chem. Sci.* **8**, 3192 (2017). [https://doi.org/10.6084/m9.figshare.c.3846712]

[2] Justin S. Smith, Ben Nebgen, Nicholas Lubbers, Olexandr Isayev, Adrian E. Roitberg. "Less is more: Sampling chemical space with active learning" *J. Chem. Phys.* **148**, 241733 (2018). [https://doi.org/10.1063/1.5023802]

[3] Justin S. Smith, Benjamin T. Nebgen, Roman Zubatyuk, Nicholas Lubbers, Christian Devereux, Kipton Barros, Sergei Tretiak, Olexandr Isayev, Adrian Roitberg "Outsmarting quantum chemistry through transfer learning" *ChemRxiv* (2018). [https://doi.org/10.26434/chemrxiv.6744440.v1]

[4] Justin S. Smith, Benjamin T. Nebgen, Roman Zubatyuk, Nicholas Lubbers, Christian Devereux, Kipton Barros, Sergei Tretiak, Olexandr Isayev, Adrian Roitberg "Approaching coupled cluster accuracy with a general-purpose neural network potential through transfer learning" *Nat. Commun.* **10,** 2903 (2019). [https://doi.org/10.1038/s41467-019-10827-4]

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3rd Annual Hands-On with Molecular Simulation Workshop

3rd Annual Hands-On with Molecular Simulation
8am-3pm November 10 at the 2019 AIChE Annual Meeting

Join us for Hands-On with Molecular Simulation Workshop from 8am-3pm on Sunday November 10th! Now in its third year, this workshop is tailored to help students, postdocs, and faculty get more research done, more reproducibly, with less pain. Hands-on tutorials designed by scientific software developers provide accessible introductions to molecular dynamics and Monte Carlo tools including MoSDEF, HOOMD, GOMC, and FEASST, with overlapping themes of reproducible scientific workflows, model creation, and coarse-graining. This year's tutorials are led by the Cummings, McCabe, Glotzer, Potoff, Jankowski, and Hatch labs.

This event is an excellent way to find your fit in the simulation community, and the workshop materials distributed via virtual machine will help you stay engaged, building off workshop conversations and demonstrations. Registration is added during AIChE annual meeting registration, costs $150 (this is a new AIChE workshop policy) and supports CoMSEF activities. For more information email ericjankowski@boisestate.edu or ssarupr@g.clemson.edu.

Day	Date	Annual Meeting Sessions	Time	Location (all in Hyatt Regency Orlando)	Co-listed
Sun	Nov 10	08A03 Atomistic and Molecular Modeling and Simulation of Polymers	3:30 PM - 6:00 PM	Celebration 8	X
		T3005 Reaction Path Analysis Using Advanced Data Science Methods	3:30 PM - 6:00 PM	Peacock Spring	X
Mon	Nov 11	08A10 Multiscale and Coarse-Grained Modeling of Polymers	8:00 AM - 10:30 AM	Celebration 15	X
		01A06 Faculty Candidates in CoMSEF/Area 1a	8:00 AM - 10:30 AM	Peacock Spring	X
		21003 Applications of Molecular Modeling to Study Interfacial Phenomena I	8:00 AM - 10:30 AM	Rock Spring I/II	
		26007 Computational Solid State Pharmaceutics	12:30 PM - 3:00 PM	Celebration 7	X
		T3000 Plenary: Topical Conference in Molecular and Materials Data Science	12:30 PM - 3:00 PM	Peacock Spring	X
		21007 Software Engineering in and for the Molecular Sciences	12:30 PM - 3:00 PM	Rock Spring I/II	
		01A01 Spotlights in Thermodynamics and Computational Molecular Science (Invited Talks)	12:30 PM - 3:00 PM	Silver Spring I/II	X
		T3002 Applications of Data Science in Molecular Sciences I	3:30 PM - 6:00 PM	Peacock Spring	X
		21006 Recent Advances in Molecular Simulation Methods I	3:30 PM - 6:00 PM	Rock Spring I/II	
		Molecular Simulation Garden Party	6:00 PM - 7:00 PM		X
Tue	Nov 12	T3001 Applications of Data Science in Catalysis and Reaction Engineering I	8:00 AM - 10:30 AM	Peacock Spring	X
		21009 Applications of Molecular Modeling to Study Interfacial Phenomena II	8:00 AM - 10:30 AM	Rock Spring I/II	
		T3003 Data-Driven Design and Modeling of Biomaterials	12:30 PM - 3:00 PM	Peacock Spring	X
		21001 Industrial Applications of Computational Chemistry and Molecular Simulation (Invited Talks)	12:30 PM - 3:00 PM	Rock Spring I/II	
		01A15 Thermophysical Properties and Phase Behavior	12:30 PM - 3:00 PM	Silver Spring I/II	X
		21002 Poster Session: Computational Molecular Science and Engineering Forum	3:30 PM - 5:00 PM	Regency Ballroom R/S	
Wed	Nov 13	T3006 Applications of Data Science in Catalysis and Reaction Engineering II	8:00 AM - 10:30 AM	Peacock Spring	X
		20031 New Methods and Developments in Computational Catalysis I	8:00 AM - 10:30 AM	Plaza International Ballroom F	X
		21010 Recent Advances in Molecular Simulation Methods II	8:00 AM - 10:30 AM	Rock Spring I/II	
		18A00 Data Science Education in Chemical Engineering Panel Discussion	12:30 PM - 3:00 PM	Manatee Spring I	X
		T3007 Applications of Data Science in Molecular Sciences II	12:30 PM - 3:00 PM	Peacock Spring	X
		21005 Practical Applications of Computational Chemistry and Molecular Simulation I	12:30 PM - 3:00 PM	Rock Spring I/II	
		18A01 CACHE 50th Anniversary: The Future of Cyber-Assisted Chemical Engineering Education	3:30 PM - 6:00 PM	Regency Ballroom T	X
		21000 Forum Plenary: Computational Molecular Science and Engineering Forum (Invited Talks)	3:30 PM - 6:00 PM	Rock Spring I/II	
		01A09 Mesoscale Modeling Advances for Thermodynamics, Transport and Reaction	3:30 PM - 6:00 PM	Silver Spring I/II	X
Thu	Nov 14	20012 Catalysis for Biomass Upgrading I: Reaction Fundamentals	8:00 AM - 10:30 AM	Florida Ballroom B	X
		20019 Confluence of Experimental and Theoretical Methods	8:00 AM - 10:30 AM	Plaza International Ballroom F	X
		21012 Recent Advances in Interfacial and Nano Particle Simulation Methods	8:00 AM - 10:30 AM	Rock Spring I/II	
		01A13 Thermodynamics Needs of the Chemical Industry	8:00 AM - 10:30 AM	Silver Spring I/II	X
		20042 Catalysis for Biomass Upgrading II: Novel Catalytic Materials	12:30 PM - 3:00 PM	Florida Ballroom B	X
		01A07 Gas Hydrates Science and Engineering	12:30 PM - 3:00 PM	Peacock Spring	X
		21011 Practical Applications of Computational Chemistry and Molecular Simulation II	12:30 PM - 3:00 PM	Rock Spring I/II	
		01A00 New Frontiers of Molecular Thermodynamics (Invited Talks)	12:30 PM - 3:00 PM	Silver Spring I/II	X
		21004 Making Molecular Simulation a Mainstream Chemical Engineering Tool	3:30 PM - 6:00 PM	Rock Spring I/II	
Fri	Nov 15	21008 The Industrial Fluid Properties Simulation Challenge	8:00 AM - 10:30 AM	Celebration 2	
		01A08 Inverse Design of Soft Materials	12:30 PM - 3:00 PM	Celebration 2	X

Upcoming Conferences of Interest to CoMSEF Members

34th Molecular Modelling Workshop 2020
Erlangen, GER
February 17-19, 2020
https://mmws2020.mgms-ds.de/

4th Conference on Multiscale Modelling of Condensed Phase and Biological Systems - CCPBioSim & CCP5
Manchester, UK
March 30-April 1, 2020
http://www.ccpbiosim.ac.uk/events/upcoming/eventdetail/123/-/4th-conference-on-multiscale-modelling-of-condensed-phase-and-biological-systems-ccpbiosim-ccp5

31st European Symposium on Applied Thermodynamics
Paris, France
June 28-July 1, 2020
http://www.esat2020.com/

Gordon Conference: Computational Chemistry
Castelldefels, Spain
July 19-24, 2020
https://www.grc.org/computational-chemistry-conference/2020/

11th Liquid Matter Conference
Prague, Czech Republic
July 20-24, 2020
http://www.lmc2020.cz/

Gordon Conference: Computational Materials Science and Engineering
Newry, ME
August 2-7, 2020
https://www.grc.org/computational-materials-science-and-engineering-conference/2020/

Why CoMSEF?

Occasionally it is worthwhile to remind everyone what CoMSEF does for our community and why your membership support is important. CoMSEF was founded in 2000, and since that time it has worked to advance molecular science and engineering in diverse ways:

* We provide a forum for communication and networking within the community. The document you're reading now is a prime example, but there is more. The annual membership meeting provides a venue for communication and interaction among members. The CoMSEF web site http://comsef.org is another useful resource for this purpose. It often hosts notices about upcoming workshops, available post-doc positions, etc.

* We provide a vehicle for communication and advocacy for molecular science and engineering in relation to other research communities. For example, our four Liaison Directors identify opportunities for co-sponsorship of sessions at the AIChE Annual Meeting, facilitate programming with other organizations, and communicate and advocate CoMSEF activities with other organizations.

* We help to recognize and promote outstanding researchers and promising graduate students by funding and administering several awards. Most recently we initiated the Young Investigator Award for Modeling and Simulation. This and our other awards help the contributions of some of our best researchers to be recognized by a broad audience, extending into the larger chemical engineering community. Your dues make these awards possible.

* We provide technical programming support, ensuring we have sessions of interest to you at the AIChE meeting. These include the many sessions we sponsor or co-sponsor, as well as the CoMSEF plenary, CoMSEF poster, and Industrial Fluid Properties Simulation Challenge sessions. We also work externally to AIChE, providing technical sponsorship to conferences in our discipline (e.g., FOMMS), where we help to ensure that these events have molecular science and engineering content of the highest quality.

Your support of CoMSEF through your membership is very important in enabling us to fulfill our mission. The financial element is valuable of course, but we also gain strength in demonstrating the size of the community we represent. So please make sure to check the box to include renewal of your CoMSEF membership whenever you pay your annual dues to AIChE. When the opportunity arises, encourage your non-member colleagues in the molecular science and engineering community to join too!