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/

Newsletter

AIChE

November 2021

In This Issue

Jayaraman Winner of 2021 CoMSEF Impact Award

Professor Arthi Jayaraman from the Department of Chemical and Biological Engineering at the University of Delaware is the winner of the 2021 CoMSEF Impact Award. She is cited "***for outstanding developments in modeling, theory, and simulation of polymer blends, nanocomposites, solutions, and biomaterials critical to the engineering design of advanced materials.***" Prior to joining the faculty at Delaware in 2019, Arthi was a professor in the Department of Chemical and Biological Engineering at the University of Colorado at Boulder. She received her PhD from North Carolina State University in 2006 with Carol Hall. For her post-doctoral research, she worked with Kenneth Schweizer in the Department of Materials Science and Engineering at University of Illinois-Urbana Champaign. She was also the winner of the inaugural CoMSEF Young Investigator Award for Modeling and Simulation in 2013. Arthi will deliver a presentation describing her research during the CoMSEF Plenary Session at the 2021 AIChE Annual Meeting. The CoMSEF Impact Award is given annually to a CoMSEF member who is within 15 years of completion of their highest degree.

Van Lehn Winner of the 2021 CoMSEF Young Investigator Award

Professor Reid C. Van Lehn from the Department of Chemical and Biological Engineering at the University Wisconsin-Madison is the 2021 winner of the CoMSEF Young Investigator Award. He is cited "***for the development and application of computational techniques to understand the interfacial properties of functionalized nanomaterials and their interactions with lipid membranes***." Reid joined the faculty at Wisconsin in 2016. Before that he worked with Professor Thomas F. Miller III at the California Institute of Technology and with Professor Alfredo Alexander-Katz at the Massachusetts Institute of Technology as a Post-doctoral researcher. Reid received his PhD in Materials Science and Engineering from the Massachusetts Institute of Technology in 2014 with Professor Alexander-Katz. Reid will deliver a presentation describing his research during the CoMSEF Plenary Session at the 2021 AIChE Annual Meeting. The CoMSEF Young Investigator Award is given annually to a CoMSEF member who is within 7 years of completion of their highest degree.

2021 CoMSEF Graduate Student Awards

The CoMSEF Graduate Student Awards in Computational Molecular Science and Engineering will be awarded after the AIChE Annual Meeting in Boston. 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 (either in person or virtual).

CoMSEF Elections

The annual CoMSEF election is currently underway and will select two liaison directors who:

- Facilitate programming with other organizations by identifying opportunities for co-sponsorship
- Communicate and advocate CoMSEF activities with other organizations.
- As members of the Executive Committee, aid the other officers in developing and carrying out CoMSEF activities and preparing the CoMSEF newsletter.

CoMSEF Business Meeting in Boston

CoMSEF will hold its annual General Meeting on Wednesday November 10 from 6:15-7:15 pm in in Marriott, Salon J/K. As in the past, the meeting will be held jointly with Area 1a (Thermodynamics and Transport Properties). All CoMSEF members are encouraged to attend.

A Broader View: Resilience at the Interface

Mona Minkara & Elizabeth Janney, Northeastern University

My research as a computational chemist tells stories of resilience that interweave with my personal narrative as a blind scientist. As a chemist, I use computational methods to study pulmonary surfactant. Pulmonary surfactant is a complex lipid-protein mixture that lines the alveoli in the lungs and is essential for proper lung function through its ability to regulate the surface tension of the air-water interface. The process of breathing is remarkably resilient.

As we inhale, the alveoli in our lungs expand and pulmonary surfactant must adapt by reaching new stability at the interface. In addition, as we breathe in, foreign entities enter through our airways. Pulmonary surfactant must fight against these pathogens while trying to find stability. Then, as we exhale, the alveoli in our lungs contract, and pulmonary surfactant is forced again to adapt. Breathing is a sustained process of resilience - of reaching new stable states.

I grew up as a Muslim girl in a mostly white neighborhood. I was a blind student among sighted classmates. I loved science and experiments - Bill Nye, Sherlock Holmes, and the Magic School Bus. I did not blend in. More so, I did not easily fit into the public system of education. I was bored with my special education placement. I did not have outlets to pursue discovery or ask the kinds of questions I needed to explore. I reached my modulus of resilience right before my sophomore year in high school and decided I would take Advanced Biology.

In science, resilience is the ability of a material to withstand elastic deformation without deforming plastically. In other words, resilience involves the stretching of atomic bonds before the breaking of the bonds. The maximum amount of volume that a material will elastically deform before becoming permanently deformed is known as the modulus of resilience.[1]

When the high school science teacher advised against taking Advanced Biology, telling me I would fail the class and should instead remain in my placement, I found my voice. I began to advocate for myself. I had a right to advanced STEM classes. My parents were taxpayers. I had the right to try and to fail. I began testing perceived limits.

The moment I remember, the moment where I grew into a new resilience was not in the struggle at the interface standing up for my right to a STEM education, but after. I excelled in the Advanced Biology course. I proved to myself that I could do advanced science. The experience enabled me to overcome the constructs holding me back. I found that the strength of my curiosity naturally dispels any fear.

"Nothing in life is to be feared, it is only to be understood. Now is the time to understand more, so that we may fear less." (Madame Curie, "La vita non è facile, e allora? Lettere di un genio forte e curioso," 2015)

As a postdoctoral researcher at the University of Minnesota's Chemical Theory Center, my advisor reframed my disability as a strength: "I have seen how you do your research. I see that you think outside of the box. We need people like you to solve the problems that no one else has." It felt like pieces of a puzzle coming together - like leveling up. Instead of blindness being a narrative of lack, I learned I had something powerful to give. My disability, my difference could be a strength. It is this kind of new stability, this resilience, that we must find in each other and build together.

Allowing difference to flourish and engage ideas in new ways could lead to answers to some of our most challenging human problems. Diversity and inclusivity are not only good for scientists; this is also very good for science. When you do not prejudge who is capable, the outcome is naturally diverse. We do not lack people who want to do science. We lack opportunities.

This is the beauty of the interface. An interface marks two spatial regions occupied by different matter or by matter in different physical states. Reactions at the interface are both incredibly important and remarkably difficult. Like the moment I chose to take Advanced Biology, or when our lungs expand and pathogens enter, or when we breath. The reaction at the interface is an opportunity for science to discover new and diverse forms of resilience.

[1] Corrosionpedia, "What is resilience," 2017

Research Highlight: Computational approaches to tackle the plastics problem

Poornima Padmanabhan, Chemical Engineering, Rochester Institute of Technology

The production, use, and fate of all plastics ever made[1] tells a grim and compelling story. Tackling the plastics problem could be approached by a number of divergent methods ranging from the development of specific catalysts for recycling and reuse, to understanding the fundamental mechanisms of degradation for current plastics already in the environment, to the use of data-driven approaches for understanding trends in large classes of plastics[2] that can inform public policy. Over the past few decades, molecular simulations have made significant contributions by providing insights to the degradation of polymers.

To study thermal degradation through bond scission, early studies utilized a Morse potential to describe atomic bonds, which enabled dynamic bond formation and breakage throughout the simulation. This technique offered insights into the role of secondary structure of the polymers, and produced temperature-dependent behavior in agreement with experimental data.[3,4] In the past two decades, the ReaxFF force-field, a bond-order based potential that accounts for dynamic bond formation and breakage, has led to greater improvements in the accuracy of these potentials, benchmarked against predictions from first-principles. The applicability of ReaxFF potentials[5] under extreme environments such as high temperatures and under high mechanical stresses can also offer insights into multiple mechanisms of polymer degradation. Several polymer chemistries have been studied using ReaxFF including polydimethylsiloxane, polyethylene, polycarbonates, and rubbers, offering novel insights in some cases.[6–9] A study of polydimethylsiloxane (PDMS) degradation at high temperatures and pressures suggested that addition of more reactive species such as ozone can lower degradation temperature;[6] another study of the degradation of polyethylene (PE) suggests that bond-breakage does not occur via random scission, but that recombination of molecular fragments to form branched polymers plays a role.[7]

Most reactions using the traditional ReaxFF potential are studied at extreme (high) temperatures because the timescale limitations in these fully atomistic simulations do not allow exploration of timescales beyond a few nanoseconds. Thus, the temperature ramp rates may be irrelevant to environmental conditions of interest. Recently, accelerated reactive molecular dynamics was developed[10,11] to study the activation energy of specific reactions at room temperature. In this method, a biasing potential is applied at a predefined rate to tagged atoms participating in the reaction, enabling them to cross the reaction barrier. The biasing potential can be chosen to stretch bonds (for breakage) and compress bonds (for formation). Accelerated ReaxFF was applied to study the hydrolysis of citrate-based polymers and provides a method to obtain activation energies for the hydrolysis of different functional groups. Additionally, non-equilibrium strain sweeps were able to identify the strength of the materials after they underwent partial or complete hydrolysis, making a valuable connection between the mechanical strength and the chemical state. Such accelerated techniques enable the study of polymer processing and rheology coupled with their degradation at *room temperature*, providing insights into the processability of plastics.

1. Geyer, R., Jambeck, J. R. & Law, K. L. Production, use, and fate of all plastics ever made. *Sci. Adv.* **3**, e1700782 (2017).
2. Min, K., Cuiffi, J. D. & Mathers, R. T. Ranking environmental degradation trends of plastic marine debris based on physical properties and molecular structure. *Nat. Commun.* **11**, 727 (2020).
3. Nyden, M. R. & Noid, D. W. Molecular dynamics of initial events in the thermal degradation of polymers. *J. Phys. Chem.* **95**, 940–945 (1991).
4. Stoliarov, S. I., Westmoreland, P. R., Nyden, M. R. & Forney, G. P. A reactive molecular dynamics model of thermal decomposition in polymers: I. Poly(methyl methacrylate). *Polymer (Guildf).* **44**, 883–894 (2003).
5. Senftle, T. P. *et al.* The ReaxFF reactive force-field: development, applications and future directions. *npj Comput. Mater.* **2**, 15011 (2016).
6. Chenoweth, K., Cheung, S., van Duin, A. C. T., Goddard, W. A. & Kober, E. M. Simulations on the Thermal Decomposition of a Poly(dimethylsiloxane) Polymer Using the ReaxFF Reactive Force Field. *J. Am. Chem. Soc.* **127**, 7192–7202 (2005).
7. Lane, J. M. D. & Moore, N. W. Molecular and Kinetic Models for High-Rate Thermal Degradation of Polyethylene. *J. Phys. Chem. A* **122**, 3962–3970 (2018).
8. Zhao, T., Li, T., Xin, Z., Zou, L. & Zhang, L. A ReaxFF-Based Molecular Dynamics Simulation of the Pyrolysis Mechanism for Polycarbonate. *Energy & Fuels* **32**, 2156–2162 (2018).
9. Saha, T. & Bhowmick, A. K. Influence of nanofiller on thermal degradatino resistance of hydrogenated nitrile butadiene rubber. *Rubber Chem. Technol.* **92**, 263–285 (2018).
10. Vashisth, A., Ashraf, C., Zhang, W., Bakis, C. E. & van Duin, A. C. T. Accelerated ReaxFF Simulations for Describing the Reactive Cross-Linking of Polymers. *J. Phys. Chem. A* **122**, 6633–6642 (2018).
11. Dasgupta, N., Yilmaz, D. E. & van Duin, A. Simulations of the Biodegradation of Citrate-Based Polymers for Artificial Scaffolds Using Accelerated Reactive Molecular Dynamics. *J. Phys. Chem. B* **124**, 5311–5322 (2020).

Where are They Now?

Now that CoMSEF has been giving the graduate student awards for more than 10 years, we've started including a "where are they now?" section in the newsletter, catching up with the winners from ~ 10 years ago.

Lauren Abbott
2011 Grad Student Award winner (Penn State University, Advisor: Coray Colina)
Poster Title: Molecular Simulations of Network Polymers of Intrinsic Microporosity: Structure Generation by a Simulated Polymerization Algorithm and Gas Adsorption Studies

Lauren received a PhD in Materials Science and Engineering in 2013, under advisement of Prof. Coray Colina at The Pennsylvania State University. Lauren was then a postdoctoral researcher for about 3 years at Sandia National Laboratories in Albuquerque, working mainly with Drs. Mark Stevens and Amalie Frischknecht. There, Lauren primarily studied temperature-responsive polymers and polymer electrolytes for proton exchange membranes. Since 2017, Lauren has been working in the Thermal Protection Materials Branch at the NASA Ames Research Center, as a member of a small computational materials modeling group. Lauren has had the pleasure to work on a variety of materials for all sorts of NASA applications, including ablative heat shield composites for atmospheric entry systems, aerospace composites for airframes, high-temperature materials for thermal propulsion systems, and polymer electrolytes for advanced battery technologies.

Upcoming Conferences of Interest to CoMSEF Members

Supercomputing 21
St. Louis, MO
November 14-19, 2021
https://sc21.supercomputing.org/

PPEPPD
Tarragona, Spain
May 22-26, 2022
https://ppeppd.org/

8th Annual CCPBioSim Conference - Frontiers in Biomolecular Simulation 2022
Edinburgh, Scotland
June 6-8, 2022
LINK

ICCT 2022
International Conference on Chemical Thermodynamics
Copenhagen, Denmark
June 9-10, 2022
LINK

Molecular Simulation 2020: Present, Past and Future
Erice, Italy
July 2022
https://bricabrac.fisica.unimo.it/ErcMlk80/

FOMMS
Delavan, WI
July 17-22, 2022
http://fomms.org

Computational Chemistry Gordon Research Conference
Castelldefels, ES
July 17-22, 2022
LINK

Polymer Physics Gordon Research Conference
South Hadley, MA
July 24-29, 2022
https://www.grc.org/polymer-physics-conference/2022/

Computational Materials Science and Engineering Gordon Research Conference
Newry, ME
July 31-August 5, 2022
LINK

STATPHYS28
Tokyo, Japan
August 8-12, 2022
https://statphys28.org/

17th International Conference of Quantum Chemistry
Bratislava, Slovakia
June 26-July 1, 2023
https://icqc2023.org/

CoMSEF Sessions at the AIChE Annual Meeting

Date	Session	Time	Location
November 7	21012 Software Engineering in and for the Molecular Sciences	3:30 PM - 6:00 PM	Marriott, Salon J/K
	01A12 Rational Design and Optimization of Soft Materials	3:30 PM - 6:00 PM	Marriott, Salon A/B
	T3001 Applications of Data Science in Catalysis and Reaction Engineering I	3:30 PM - 6:00 PM	Marriott, Salon H/I
November 8	21001 Spotlights in Thermodynamics and Computational Molecular Science (Invited Talks)	8:00 AM - 10:30 AM	Marriott, Salon J/K
	T5000 Advanced batteries I	8:00 AM - 10:30 AM	Hynes CC, 306
	T3003 Applications of Data Science in Molecular Sciences I	8:00 AM - 10:30 AM	Marriott, Salon H/I
	21005 Data-Driven Design and Modeling I	12:30 PM - 3:00 PM	Marriott, Salon J/K
	01A07 Faculty Candidates in CoMSEF/Area 1a, Session 1	12:30 PM - 3:00 PM	Marriott, Salon A/B
	T5004 Plasma catalysis	12:30 PM - 3:00 PM	Hynes CC, 306
	T3005 Applications of Data Science to High Throughput Experimentation	12:30 PM - 3:00 PM	Marriott, Salon H/I
	21006 Data-Driven Design and Modeling II	3:30 PM - 6:00 PM	Marriott, Salon J/K
	02E15 Molecular and Data Science Modeling of Adsorption I	3:30 PM - 6:00 PM	Hynes CC, 110
	T5003 Perovskites, spinels, energy conversion, modeling of these systems	3:30 PM - 6:00 PM	Hynes CC, 306
	01A08 Faculty Candidates in COMSEF/Area 1a, Session 2	3:30 PM - 6:00 PM	Marriott, Salon A/B
	T3006 Innovations in Methods of Data Science	3:30 PM - 6:00 PM	Marriott, Salon H/I
November 9	21007 Nanoscale Behavior of Sustainable Processes	8:00 AM - 10:30 AM	Marriott, Salon J/K
	T5002 Hybrid systems, halide perovskites, molecular modeling	8:00 AM - 10:30 AM	Hynes CC, 306
	01A14 Special Session In Honor of Arup Chakraborty's 60th Birthday: Statistical Mechanics and Molecular/Materials Modeling	8:00 AM - 10:30 AM	Marriott, Salon C/D
	T3000 Topical Plenary: Topical Conference in Molecular and Materials Data Science (Invited Talks)	8:00 AM - 10:30 AM	Marriott, Salon H/I
	21011 Recent Advances in Multiscale Methodologies	12:30 PM - 3:00 PM	Marriott, Salon J/K
	T5005 Soft systems, molecular simulation, sustainability	12:30 PM - 3:00 PM	Hynes CC, 306
	01A13 Special Session In Honor of Arup Chakraborty's 60th Birthday: Biology and Immunology	12:30 PM - 3:00 PM	Marriott, Salon C/D
	T3002 Applications of Data Science in Catalysis and Reaction Engineering II	12:30 PM - 3:00 PM	Marriott, Salon H/I
	21002 Poster Session: Computational Molecular Science and Engineering Forum (CoMSEF)	3:30 PM - 5:00 PM	Hynes CC, Exhibit Hall C/D
	T5001 Advanced batteries II	3:30 PM - 5:00 PM	Hynes CC, 306
	T3004 Applications of Data Science in Molecular Sciences II	3:30 PM - 5:00 PM	Marriott, Salon H/I
November 10	21008 Practical Applications of Computational Chemistry and Molecular Simulation I	8:00 AM - 10:30 AM	Marriott, Salon J/K
	T4003 Teaching Data Science to Students and Teachers I	8:00 AM - 10:30 AM	Hynes CC, 306
	21009 Practical Applications of Computational Chemistry and Molecular Simulation II	12:30 PM - 3:00 PM	Marriott, Salon J/K
	T4004 Teaching Data Science to Students and Teachers II	12:30 PM - 3:00 PM	Hynes CC, 306
	21000 Plenary Session: Computational Molecular Science and Engineering Forum (Invited only)	3:30 PM - 6:00 PM	Marriott, Salon J/K
	02E17 Molecular Simulations for Designing Adsorbents and Adsorption Processes I	3:30 PM - 6:00 PM	Hynes CC, 305
	01A03 Computational Studies of Early-Stage and Low-Dimensional Self-Assembly	3:30 PM - 6:00 PM	Marriott, Salon H/I
November 11	21010 Recent Advances in Molecular Simulation Methods	8:00 AM - 10:30 AM	Marriott, Salon J/K
	21003 Applications of Molecular Modeling to Study Interfacial Phenomena I	12:30 PM - 3:00 PM	Marriott, Salon J/K
	21004 Applications of Molecular Modeling to Study Interfacial Phenomena II	3:30 PM - 6:00 PM	Marriott, Salon J/K
	01A05 Development of Intermolecular Potential Models	3:30 PM - 6:00 PM	Marriott, Salon H/I
November 15	T4005 Teaching Data Science to Students and Teachers III	8:00 AM - 10:40 AM	Virtual, Bridging the Skills Gap in Chemical Engineering (T4)
	21013 CoMSEF Poster Session - Virtual	10:30 AM - 12:00 PM	Virtual, Posters
	02E16 Molecular and Data Science Modeling of Adsorption II	12:30 PM - 3:00 PM	Virtual, Separations Division (02)
	02E18 Molecular Simulations for Designing Adsorbents and Adsorption Processes II	3:30 PM - 6:00 PM	Virtual, Separations Division (02)
November 16	21015 Recent Advances and Applications of Molecular Modeling Virtual	8:00 AM - 10:30 AM	Virtual, Computational Molecular Science and Engineering Forum (21)
	21016 Practical Applications of Computational Chemistry and Molecular Simulation III	12:30 PM - 3:10 PM	Virtual, Computational Molecular Science and Engineering Forum (21)
	21014 Data-Driven Design and Modeling Virtual	3:30 PM - 6:00 PM	Virtual, Computational Molecular Science and Engineering Forum (21)
November 18	T4002 Practical Application of Process Data Analytics and Machine Learning (Invited Talks)	8:00 AM - 10:30 AM	Virtual, Bridging the Skills Gap in Chemical Engineering (T4)

FOMMS 2022

The Foundations of Molecular Modeling and Simulation (FOMMS) meeting will be held July 17-21, 2022 at The Lake Lawn resort in Delavan, WI (85 miles northwest from Chicago O'Hare airport and 50 miles southwest from Milwaukee Mitchell airport). The meeting was postponed one year due to the pandemic. FOMMS 2022 will be the eighth triennial FOMMS conference showcasing new developments and applications of computational quantum chemistry, statistical mechanics, molecular simulation and theory, and continuum and engineering process simulation. The theme of the meeting is “Molecular Modeling and the Data Revolution”. The meeting will feature eighteen invited talks by leading experts clustered around the following themes

Applications of Machine Learning
Biological Systems
Energy and environment
Molecular Modeling Fundamentals
New Approaches in Computational Catalysis
Product Design
Sustainability

In addition, there will be an opening plenary lecture and the meeting will conclude with the traditional FOMMS Medal recipient. We are pleased to announce that Doros Theodorou of the National Technical University of Athens was selected as the 2022 FOMMS Medal recipient. The meeting will also feature two poster sessions for contributed papers and hands-on workshops. An optional outing can be taken by participants to enjoy the surroundings one afternoon.

More information may be found at the conference website fomms.org.

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!