School of Molecular Sciences
Arizona State University

SMS Fall 2023 Seminar Series

Friday October 6 | 3pm | Biodesign Auditorium

Machine Learning in Chemistry: Cheap and Accurate Energies and Forces in molecular systems. Uses in conformational searches and free energy calculations.

In the theoretical study of molecular systems, a compromise between speed and accuracy is required to study the energetics of chemical systems. Quantum mechanical (QM) methods allow accurate energies and forces to be calculated but require massive computational effort. Classical force fields are fast but only accurate near equilibrium and are generally unusable in reactivity studies due to restrictive functional forms or man hour intensive parametrization. One solution to these problems is the development of empirical potentials, however, little progress has been made towards accurate and general purpose empirical models. Machine learning methods such as artificial neural networks have been used to develop neural network potentials (NNP), which are fit to QM reference energies, though few have shown to be size extensible. Through the continued development of our methodology and data set, known as ANAKIN-ME (or ANI for short), we developed a new class of NNP, which is size extensible and chemically accurate. Specifically, we develop the ANI potential for organic molecules containing H, C, N, O, F, S, and Cl. Through extensive benchmarks, case studies, and molecular dynamics simulations, we will provide evidence that the ANI method produces chemically accurate and size extensible potentials. As the results clearly show, the ANI method is a potential game changer for molecular simulation. The ANI method continues to bring a new, highly efficient, and accurate method for the development of NNPs into the realm of reality, and opens the door for the next generation of “out-of-the-box” general purpose potentials.

Adrian Roitberg

Professor, University of Florida

Prof. Adrian Roitberg was born and raised in Buenos Aires Argentina, where he received his BS in Chemistry from the University of Buenos Aires. He moved to the US in 1989, where he received his PhD in Theoretical Physical Chemistry at the University of Illinois at Chicago in 1992, working with Prof. Ron Elber. His work at that time focused on molecular dynamics of biomolecules. He then spent 3 years as a postdoctoral fellow at Northwestern University in Evanston, IL, working with Prof. Mark Ratner. There he worked on computing vibrational spectra for very large biomolecular systems, and was lucky enough to play a small role in the renaissance of the filed of molecular electronics, by hanging around with Vladimiro Mujica. Dr. Roitberg moved to a staff position at the National Institute for Standards and Technology in Maryland, where he worked from 1995 to 2000. In 2001, his spouse, Prof. Valeria Kleiman was recruited by the University of Florida as an Assistant Professor, and UF was generous enough to create a position for Dr. Roitberg. He rose through the ranks, and he is know the "V.T. and Louise Jackson Professor in Chemistry" at U Florida, with an affiliate appointment in the department of physics. Prof, Roitberg has published close to 200 peer-reviewed articles, has graduated 30 PhD students, and has received funding from DOE, NIH and NSF at various times. He has been the recipient of several awards, being named fellow of both the American Chemical Society and the American Physical Society, been an "Ulam Fellow" at Los Alamos National Laboratory. Near and dear to his heart, he received the Raices (roots) award from the Science Ministry of Argentina, and recently was awarded an honorary doctorate from the University of Buenos Aires.

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