

Chemistry Colloquium

Wednesday, October 20, 12 pm

Hutchison Hall, Lander Auditorium

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“Machine Learning for Accurate Energies and Forces in molecular systems. Uses in conformational searches and free energy calculations”

Abstract: 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.



Website: https://events.rochester.edu/event/chemistry_physical_colloquium_roitberg

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