APS Scientific Computation Seminar Series

Speaker: Chris Benmore, Physicist
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Title: Modeling PDF data from liquids: What's next?

Date: Monday, January 31, 2022

Time: 1:00 p.m. (Central Time)

Location: **Join ZoomGov Meeting**
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Abstract: It is 89 years since Bernal and Fowler reported the first ball and stick model of water based on x-ray diffraction data. This talk covers a brief perspective of how modeling x-ray and neutron Pair Distribution Function (PDF) data from liquids and glasses has evolved since. From Lennard-Jones classical molecular dynamics potentials, to AIMD simulations that allow a full quantum mechanical description of the interatomic forces involved. However, the agreement between experimental PDFs and MD simulations are often qualitative. Quantitative agreement between model and experiment was addressed with the development of Reverse Monte Carlo methods in the late 80's and Empirical Potential Structure Refinement in the late 90's. These approaches enable "perfect" agreement to be obtained between a 3D model arrangement of atoms or molecules and the diffraction data, but they still lack an understanding of the underlying physics, or conformation that the structures are even chemically realistic! Today, machine learning has the potential to bridge this divide, and provide large scale atomistic models in agreement with experimental PDF data with quantum mechanical accuracy. This has been demonstrated through the use of active learning methods and Gaussian Approximation Potentials to develop multiphase machine learning potentials. The latest developments underscore more than ever the importance of extracting high quality experimental structure factors, which is often overlooked in some modern data PDF analysis routines designed for high-throughput data-processing.