Predicting Virial Coefficients and Alchemical Transformations by Extrapolating Mayer-Sampling Monte Carlo Simulations

Harold Hatch [C, S]
Chemical Sciences Division, NIST, Gaithersburg, MD, U.S.A.
harold.hatch@nist.gov

Sally Jiao
Chemical and Biological Engineering, Princeton University, Princeton, NJ, U.S.A.

Nathan Mahynski
Chemical Sciences Division, NIST, Gaithersburg, MD, U.S.A.

Marco Blanco
Institute for Bioscience and Biotechnology Research, University of Maryland, Rockville, MD, U.S.A.

Vincent Shen
Chemical Sciences Division, NIST, Gaithersburg, MD, U.S.A.

Virial coefficients are predicted over a large range of both temperatures and model parameter values (e.g., alchemical transformation) from an individual Mayer-sampling Monte Carlo simulation by statistical mechanical extrapolation. With this extrapolation method, a Mayer-sampling Monte Carlo simulation of SPC/E water quantitatively predicted the second virial coefficient as a continuous function spanning over four orders of magnitude in value and over three orders of magnitude in temperature with less than a 2 % deviation. In addition, the same simulation accurately predicted the second virial coefficient if the site charges were scaled by a constant factor, from an increase of 40 %, to a decrease of no charge at all. This method also performed well for the third virial coefficient and the exponential parameter of the Lennard-Jones fluid. This method increases the efficiency of accurately mapping virial coefficients over a range of parameters for use in applications such as prediction of protein aggregation, collapse of phase diagrams using extended corresponding states, computation of Boyle temperatures and theta solvent conditions, coarse-graining, and the fitting of models to experimental data. Example code is provided at https://github.com/usnistgov/mayer-extrapolation.