Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Equilibrium properties in the thermodynamic limit from small-sized molecular dynamics simulations[1] ROBINSON CORTES-HUERTO, KURT KREMER, RAFFAELLO POTESTIO, Max Planck Institute for Polymer Research — We present an accurate and efficient method to obtain equilibrium thermodynamic properties of bulk systems from small-sized molecular dynamics simulations by introducing finite size effects into integral equations of statistical mechanics. We validate the method by calculating thermodynamic properties of prototypical complex mixtures such as the activity coefficients of aqueous urea mixtures and the Kirkwood-Buff integrals of Lennard-Jones fluids. Moreover, our results demonstrate how to identify simulation conditions under which computer simulations reach the thermodynamic limit.

[1]Alexander von Humboldt Foundation

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Date submitted: 08 Nov 2016 Electronic form version 1.4