

Abstract Submitted
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Water-like Anomalous Properties and Polyamorphism in a Liquid with Smooth (Differentiable) Pair Interactions¹ JOEL ABRAHAM, NICOLAS GIOVAMBATTISTA, Department of Physics, Brooklyn College-CUNY, Brooklyn, NY 11210, USA — We perform molecular dynamics simulations of a system of particles interacting via a spherically symmetric, core-softened pair potential, which is a smooth version of the (non-differentiable) Jagla pair potential. Although liquid properties are extremely sensitive to the details of the pair interactions, we show that the smooth version of the Jagla potential preserves the main properties of the original model. Specifically, both pair potentials result in liquids that show (i) water-like thermodynamic and dynamical anomalous properties, as well as (ii) liquid and (iii) glass polymorphism (i.e., the presence of more than one liquid and glass form, respectively). The pressure-temperature phase diagram of our smooth potential shows, as observed in computer simulations using the Jagla model, a liquid-liquid first order transition line separating two liquid phases and ending in a critical point; such a critical point being accessible in equilibrium simulations.

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