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The Study of Solvation Effects on Thermodynamic Properties of Nanofluids Using Molecular Dynamics[1] GIANLUCA PULITI, SAMUEL PAOLUCCI, MIHIR SEN, DANIEL GEZELTER, University of Notre Dame — Liquid layering around nano-particles is proposed to be a major contributor in the surprisingly unpredictable properties of nanofluids. Equilibrium molecular dynamic simulations are presented for a water-based nanofluid with gold nano-particles. It makes use of state-of-the-art force fields to capture a broad spectrum of realistic physical phenomena. Thermodynamic properties, such as internal energy, heat capacity, enthalpy and entropy of the nanofluid are analyzed for different particle configurations. The understanding of basic thermodynamic effects in nanofluids is a stepping stone for further studies.

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