Abstract Submitted
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Properties of Nanofluids[1] GIANLUCA PULITI, SAMUEL PAOLUCCI, MIHIR SEN, University of Notre Dame — Equilibrium molecular dynamic simulations are presented for different configurations of interactions between gold metal and liquid water. It makes use of state-of-the-art potentials to capture a broad spectrum of realistic physical phenomena at the interface. Thermodynamic properties, such as internal energy, heat capacities, isothermal compressibility, and coefficient of thermal expansion of the nanofluid are currently being analyzed. Transport properties, such as mass diffusion, viscosity and thermal conductivity, are also under investigation. Some of the results obtained thus far, seems to strongly diverge from the prediction of ideal mixture theories. The understanding of basic thermodynamic and transport effects in nanofluids is a stepping stone to further studies.

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