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Liquid State Properties from *ab initio* Density Functional Theory Calculations NICOLAS BOCK, TRAVIS PEERY, ERIC CHISOLM, GIULIA DE LORENZI-VENNERI, DUANE WALLACE, Los Alamos National Laboratory, ERIK HOLMSTRÖM, RAQUEL LIZARRAGA, Instituto de Fisica, Universidad Austral, Chile — For the solid state, density functional theory (DFT) has been successfully applied to calculate material properties in a large range of materials. In the liquid state however, thermodynamic properties are calculated by molecular dynamics (MD) simulations in which the forces are calculated with DFT. These simulations are computationally significantly more expensive than comparable solid state calculations. We present a novel approach which does not rely on MD simulations, but instead uses Vibration-Transit (V-T) theory to make predictions of the thermodynamic properties of the liquid phase. This approach is computationally significantly less expensive than an MD simulation. The accuracy of this approach is demonstrated by a comparison to experiment.

Nicolas Bock
Los Alamos National Laboratory

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