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**Sesame style decomposition of KS-DFT molecular dynamics for direct interrogation of nuclear models**[1] SARAH BURNETT, University of Maryland - College Park, DANIEL SHEPPARD, KEVIN HONNELL, Los Alamos National Laboratory — A common paradigm used in the construction of equations of state is to decompose the thermodynamics into a superposition of three terms: a static lattice cold curve, a contribution from the thermal motion of the ions, and a contribution from the thermal excitation of the electrons. While statistical mechanical models for crystals provide tractable framework for the ionic contribution in the solid phase, much less is understood about the ionic contribution above the melt temperature ($C_v \approx 3R$) and how it should transition to the high-temperature limit ($C_v \sim \frac{3}{2}R$). In this work, we use the VASP Quantum Molecular Dynamics package to probe thermal ionic behavior in the liquid and to compare the results to two semi-empirical models – the Johnson model and the Chisolm high-temperature liquid model. For each temperature and density of interest, we begin by performing a full Kohn-Sham QMD simulation of the system. The average of the resulting internal energies and pressures is recorded for each particular temperature. Taking the derivative of the energy with respect to temperature using Gram polynomials returns the specific heat, $C_v$. We describe the general methodology and compare predictions for the constant volume heat capacity of Al to common ionic models.

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