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Improvements on the Murnaghan Equation of State MICHAEL MEHL, Center for Computational Materials Science, Naval Research Laboratory, Washington DC 20375-5000 — Formulas for interpolating the equation of state of a material are useful to consolidate both experimental and computational data. A good equation of state can reduce the computational effort needed to determine the equilibrium energy and to prediction phase transitions. The Murnaghan equation of state, which starts from the simple approximation that the bulk modulus of a system is linear in the pressure, is popular because it yields analytic expressions for V(P), P(V), E(V), and H(P) = E + P V. However, it has unphysical behavior as the bulk modulus approaches zero, predicting this to occur only at infinite volume, and at high pressure, where it misses the softening of B'(P). This paper presents a simple, analytic modification of B(P) which properly accounts for both regimes, and which still yields analytic behavior of the volume, pressure, energy, and enthalpy. The accuracy of the resulting equation of state is compared to the Murnaghan, Birch, and "Universal" equation of state for both simple and complex systems.

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