

Analytic Equation of State and Thermodynamic Properties of Solid FCC $C_{61}D_2$ Based on an Analytic Mean Field Approach

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Analytic expressions for the equation of state and internal energy of poly-exponential solids are derived based on the analytic mean field potential (AMFP) method. The formalism is applied to fcc $C_{61}D_2$. Two sets of potential parameters are determined by fitting the experimental compression data of $C_{61}D_2$ up to 1 GPa at 343 and 307 K, respectively. The difference between the two sets of parameters is small. Whereas the difference between the potential of the $C_{61}D_2$ molecules and that of the C_{60} molecules is fairly prominent, the conclusion is different from that in the literature, and the reason is unclear at present. The thermo-physical properties including the isothermals, thermal expansion, isochoric heat capacity, Helmholtz free energy and internal energy are calculated and analyzed. The theoretical results agree well with the experimental data available for solid $C_{61}D_2$.

Key words: AMFP; Morse Potential; Equation of State; Fullerene; Thermodynamic Properties.