Structural distortions in AlF$_3$ derived using density functional methods

L. L. Boyer, M. J. Mehl, Dan Finkenstadt, Center for Computational Materials Science, Naval Research Laboratory — The crystal structure of AlF$_3$ at high temperatures has a simple cubic lattice. Below $\sim 730$K the structure transforms to a rhombohedral ($\alpha$-phase) structure with R$3c$ symmetry, due to an unstable R$_5^-$ phonon. Density-functional based methods, from the least accurate rigid-ion model to highly-accurate all-electron Kohn-Sham models, yield the triply degenerate R$_5^-$ phonon that becomes unstable with decreasing volume at some critical volume $V_c$. Significant variations for $V_c$ and the equilibrium volume $V_0$ among the models lead to large uncertainties for the energy differences between the cubic and rhombohedral structures, indicating that present density functional models are not reliable for accurate quantitative results in this case.