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Atomic Simulations of Alane Phase Transformations and Dehydrogenation Mechanisms SUSANNE OPALKA, United Technologies Research Center, PAUL SAXE, Materials Design, Inc., OLE MARTIN LOVVIK, University of Oslo — Density functional theory atomic ground state, molecular dynamics, and direct method lattice dynamic simulations were used to mechanistically probe phase transformations between the various crystallographically refined α, α', β, and γ AlH_3 phases. Lattice dynamic predictions of the AlH_3 structures provided an ideal test case for systematically accessing the accuracy of the vibrational thermodynamic property contributions with the harmonic approximation. The predicted transformation pathways involved coordinated tilting and rotation mechanisms, similar to that observed in perovskite structures. Further simulations were conducted to elucidate the mechanism for α AlH_3 phase decomposition to the Al and H_2 products and to identify probable barriers to reversible rehydrogenation.

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