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Thermodynamic properties of calcium alanate from first-principle calculations XUEZHI KE, Department of Physics, University of Nevada, Las Vegas, NV 89154-4002, USA AND Department of Physics, East China Normal University, Shanghai 200062, CHANGFENG CHEN, Department of Physics, University of Nevada, Las Vegas, NV 89154-4002, USA, OLE MARTIN LOVVIK, Centre for Materials Science and Nanotechnology, University of Olso, P.O.Box 1126 Blindern, NO-0318, Norway AND Institute for Energy Technology — The potential hydrogen-storage material calcium alanate has been studied by density functional theory at the GGA level, and by phonon calculations using the harmonic approximation. The stability and thermodynamic properties of this system have been studied in detail.

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