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Electronic structure and equation of state of Sm_2Co_{17} from first-principles DFT+U[1] PATRICK HUANG, NICHOLAS P. BUTCH, JASON R. JEFFRIES, SCOTT K. MCCALL, Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory — Rare-earth intermetallics have important applications as permanent magnet materials, and the rational optimization of their properties would benefit greatly from guidance from ab initio modeling. However, these systems are particularly challenging for current electronic structure methods. Here, we present an ab initio study of the prototype material Sm_2Co_{17} and related compounds, using density functional theory with a Hubbard correction for the Sm $4f$-electrons (DFT+U method) and ultrasoft pseudopotentials. The Hubbard U parameter is derived from first principles [Cococcioni and de Gironcoli, PRB 71, 035105 (2005)], not fit to experiment. Our calculations are in good agreement with recent photoemission measurements at ambient pressure and the equation of state up to 40 GPa, thus supporting the validity of our DFT+U model.

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