Topological Phase Transition in the SmS Kondo Insulator under pressure

ZHI LI, JIN LI, Department of Physics, California State University Northridge, PETER BLAHA, Institute for Materials Chemistry, Vienna University of Technology, NICHOLAS KIOUSSIS, Department of Physics, California State University Northridge — Employing LDA+U electronic structure calculations we predict that SmS undergoes a topological phase transition from the trivial Kondo insulator (KI) black phase to a topological metallic gold phase under hydrostatic pressure. The underlying mechanism is the pressure-induced change of the 4f level from below to above the bottom of the 5d conduction band, leading to a df band inversion, a parity sign reversal, and the concomitant change of the topological invariant. This provides the first material realization of the topological classification of KIs proposed by Dzero et al.