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Ab initio studies of the electronic and transport properties of topological insulator-metal contacts CATALIN SPATARU, FRANCOIS LEONARD, Sandia National Laboratories — Topological insulators (TI) hold great promise for novel applications in electronics and optoelectronics. For such device applications, TIs need to be contacted with a metal for electron injection. Depending on the character and strength of the interaction, a metal contact can modify the properties of TI surface states and induce new states at the interface. In this work, we study via ab initio Density Functional Theory the electronic and transport properties of realistic interfaces between a thin film TI and several magnetic and non-magnetic metal surfaces. We will discuss how band topology, band bending and hybridization effects affect charge injection and the contact properties (Schotkky versus ohmic) of the interface.

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