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A DFT study of supported 2D-Sn (Stannanane) films ANA SUAREZ NEGREIRA, MAX FISCHETTI, University of Texas at Dallas — Theoretical studies indicated that Sn monolayer is a 2D topological insulator with robust properties against small perturbations, thus resulting in large tolerance against variations induced by a manufacturing process. The downside of many topological properties is that they manifest themselves only at very low temperatures. However, thin film of Sn have a significantly higher phase transition temperature, up to 120 °C, creating new opportunities of using this material in nano-electronics applications. Since stannanane has never been synthesized before, its existence and mechanical stability are open questions. Using density functional theory (DFT), we study the growth of stannanane on various substrates (i.e., InSb(100) and CdTe(100)). The impact of the substrate on the electronic properties of this topological insulator is studied through Bader charge and density of states (DOS) analyses. Finally, ab initio thermodynamics methodology is used to study the stability of different Sn surface terminations as a function of temperature and pressure.

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