First principles calculations of the two dimensional topological insulator stanene on substrates

STEPHEN ELTINGE, Department of Physics, Yale University, MINJUNG KIM, Department of Applied Physics, Yale University, STEPHEN ALBRIGHT, Department of Physics, Yale University, RUI PENG, KE ZOU, FRED WALKER, CHARLES AHN, SOHRAB ISMAIL-BEIGI, Department of Applied Physics, Yale University — Topological insulators are a class of materials under continued intense investigation due to their potentially robust current carrying surface or edge states. Stanene, the two dimensional form of tin, has been predicted to be a 2D topological insulator due to its large spin-orbit interaction. There exist a number of first principles calculations of stanene both as an isolated layer as well as on a substrate, but the only successful experimental report involves the growth of stanene on Bi$_2$Te$_3$, and does not show signatures of topological behavior.* In this work, we present first-principles density functional theory calculations of stanene on a Bi$_2$Te$_3$ substrate and report on the binding, interfacial structure, and role of various decorating groups (i.e., atoms or molecules binding to stanene). In addition, we will describe the possible benefits of using wide gap insulators such as CdTe as substrates.


1This work is supported by Functional Accelerated nanoMaterial Engineering (FAME).