First principles calculations of the two dimensional topological insulator stanene on substrates[1]
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— 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_2Te_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_2Te_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.
*F. Zhu, W. Chen, Y. Xu, C. Gao, D. Guan, C. Liu, D. Qian, S.-C. Zhang, and J. Jia, *Nat. Mater.* (2015).

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