Strain-tunable topological quantum phase transition in buckled honeycomb lattices

Jia-An Yan[1],* Mack A. Dela Cruz[1], Salvador Barraza-Lopez[2], and Li Yang[3]
1. Department of Physics, Astronomy, and Geosciences, Towson University, 8000 York Road, Towson, MD 21252, USA
2. Department of Physics, University of Arkansas, Fayetteville, Arkansas 72701, USA
3. Department of Physics, Washington University, St Louis, MO 63005, USA
(Dated: May 15, 2015)

Low-buckled silicene is a prototypical quantum spin Hall insulator with the topological quantum phase transition controlled by an out-of-plane electric field. We show that this field-induced electronic transition can be further tuned by an in-plane biaxial strain ε, owing to the curvature-dependent spin-orbit coupling (SOC): There is a $Z_2 = 1$ topological insulator phase for biaxial strain $|\varepsilon|$ smaller than 0.07, and the band gap can be tuned from 0.7 meV for $\varepsilon = +0.07$ up to 3.0 meV for $\varepsilon = -0.07$. First-principles calculations also show that the critical field strength E_c can be tuned by more than 113%, with the absolute values nearly 10 times stronger than the theoretical predictions based on a tight-binding model. The buckling structure of the honeycomb lattice thus enhances the tunability of both the quantum phase transition and the SOC-induced band gap, which are crucial for the design of topological field-effect transistors based on two-dimensional materials.

*Electronic address: `jiaanyan@gmail.com`