

Abstract Submitted
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Two-dimensional topological insulator molecular networks: dependence on structure, symmetry, and composition LIANG Z. TAN, STEVEN G. LOUIE, Department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — 2D molecular networks can be fabricated from a wide variety of molecular building blocks, arranged in many different configurations. Interactions between neighboring molecular building blocks result in the formation of new 2D materials. Examples of 2D organic topological insulators, that contain molecular building blocks and heavy elements arranged in a hexagonal lattice, have been recently proposed by Feng Liu and coworkers (Nano Lett., 13, 2842 (2013)). In this work, we present a systematic study of the design space of 2D molecular network topological insulators, elucidating the role of structure, symmetry, and composition of the networks. We show that the magnitude and presence of spin-orbit gaps in the electronic band structure is strongly dependent on the symmetry properties and arrangement of the individual components of the molecular lattice. We present general rules to maximize the magnitude of spin-orbit gaps and perform ab-initio calculations on promising structures derived from these guidelines. This work was supported by National Science Foundation Grant No. DMR10-1006184, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by the NSF through XSEDE resources at NICS.

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