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Quantum Anomalous Hall Insulator in Asymmetrically Functionalized Germanene CHIA-HSIU HSU, Dept of Phys, Natl Sun Yat-Sen Univ and Dept of Phys, South Univ of Sci and Tech, ZHI-QUAN HUANG, CHRISTIAN P. CRISOSTOMO, YU-MING GU, Dept of Phys, Natl Sun Yat-Sen Univ, YI-MEI FANG, SHUNQING WU, ZI-ZHONG ZHU, Dept of Phys, Xiamen Univ, LI HUANG, Dept of Phys, South Univ of Sci and Tech, FENG-CHUAN CHUANG, Dept of Phys, Natl Sun Yat-Sen Univ, HSIN LIN, Graphene Research Ctr and Dept of Phys, Natl Univ of Singapore, ARUN BANSIL, Dept of Phys, Northeastern Univ — We study the atomic structures and electronic properties of honeycomb germanene passivated asymmetrically with hydrogen and nitrogen (GeHN) atoms using first-principles electronic structure calculations. There are three atomic structures considered: planar, buckled, and inversely buckled honeycomb. We found that the inversely buckled structure is in non-magnetic insulator phase; while the buckled structure is metallic. Using spin-polarized calculations with spin-orbit coupling, GeHN in planar structure was identified to exhibit a quantum anomalous Hall (QAH) insulator phase. In order to confirm the topology of the material, we further calculated the Chern number as well as the edge states. A band connecting the conduction and the valence band was found at the edge state of zigzag GeHN nanoribbon. Our results suggest that functionalized germanene might be used in the highly sought spintronic applications based on QAH effect.

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