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arXiv:2210.12457v2 [cond-mat.mes-hall] 25 Oct 2022

Oct 25, 2022 · states would emerge, such as, the quantum anomalous Hall (QAH) state and the axion insulator state3–5. As a typical magnetic topological state, the QAH state was predicted and realized in Cr-doped (Bi,Sb)2Te3 films6,7, where the magnetism is not intrinsic but induced through the doping process. Interestingly, MnBi2Te4 and its fam-

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As in so many areas of solid-state physics, density func-tional theory (DFT)17,18 has emerged as the most powerful approach for assessing the properties of defects. DFT calcu-lations, typically carried out in a supercell geometry,6 yield reliable information about atomic structure, including all relaxations of the host atoms.

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