

Abstract Submitted
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Quantum Spin Hall Effect in Two-Dimensional Transition Metal Dichalcogenides¹ XIAOFENG QIAN, Texas A&M Univ, JUNWEI LIU, LIANG FU, JU LI, Massachusetts Institute of Technology — Quantum spin Hall (QSH) effect materials have an insulating bulk but conducting edge states that are topologically protected from backscattering by time reversal symmetry. However, the small band gap and the lack of efficient on/off switching in materials that have been identified as QSH insulators limit their applications. Here using first-principles calculations we predict a class of large-gap QSH insulators in two-dimensional transition metal dichalcogenides with 1T' structure, namely, 1T'-MX₂ with M=(W, Mo) and X=(Te, Se, S)². A structural distortion causes an intrinsic band inversion between chalcogenide-*p* and metal-*d* bands. Additionally, spin-orbit coupling opens a gap that is tunable by vertical electric field and strain. We propose a topological field effect transistor made of van der Waals heterostructures of 1T'-MX₂ and 2D dielectric layers that can be rapidly switched off by electric field through topological phase transition instead of carrier depletion.

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²Xiaofeng Qian, Junwei Liu, Liang Fu, and Ju Li, arXiv:1406.2749 (2014)

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