**Predicting topological insulators in hydrogenated transition metal dichalcogenide monolayers: A first-principles study**

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Two dimensional (2D) transition metal dichalcogenides (TMD) monolayers have currently been of immense interest in materials research because of their versatility and tunable electronic properties. In this study, we perform systematically the first-principles calculations of possible topological insulator phases on 1T and 2H MX2 monolayers, as well as the effects of hydrogenation on one or both sides of the films. With regards to structural stability, we find that Group IV(Ti, Zr, Hf)-, VI(Cr, Mo, W)-, and X(Ni, Pd, Pt)-based TMDs, respectively, adopted 1T, 2H, and 1T as their stable structures for unhydrogenated cases. However, upon hydrogenation, we observe structural phase transition from 1T to 2H for Group IV, and from 2H to 1T for Group VI, and no transition was observed for Group X. We find that for 2H TiTe2 and 1T CrTe2 with 1 hydrogen, as well as 2H PdSe2 without hydrogenation, are identified to be topological insulators with large band gaps of 0.07eV, 0.21eV and 0.23eV, respectively. These findings show that these TMDs in quantum spin Hall phase have a great potential for spintronics applications.