**Two-dimensional topological insulators upon substitutional doping of monolayer VB-VIA transitional metal dichalcogenides**

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Substitutional doping of two-dimensional transition metal dichalcogenides (TMDs) is of importance in tuning and possible enhancement of its electronic, physical and chemical properties for vast industrial applications. Here we report a systematic first-principles study of possible 2D topological insulator phases, also known as quantum spin Hall (QSH) insulator, upon halogen (Cl, Br, I) or pnictogen (P, As, Sb, Bi) substitution of monolayer group VB (V, Nb, Ta) - VIA (S, Se, Te) TMDs, including the effects of one-sided hydrogen adsorption, for both 1T and 2H crystal structures. A structural phase transition, from 2H to 1T, was observed for all the pnictogen substituted TMDs while no structural phase transition upon halogen substitution or hydrogen adsorption. Nontrivial phases were obtained upon pnictogen substitution and trivial phases upon halogen substitution and hydrogen adsorption. The topology of some transition metal dichalcogenides (TMDs) becomes nontrivial upon pnictogen substitution, demonstrating its suitability for synthesis on various substrates.