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Stable, Single-Layer MX_2 Transition-Metal Oxides and Dichalcogenides in a Honeycomb-Like Structure CAN ATACA, HASAN SAHIN, SALIM CIRACI, UNAM-National Nanotechnology Research Center, Bilkent University, Ankara 06800, Turkey — Recent studies have revealed that single-layer transition-metal oxides and dichalcogenides (MX_2) might offer properties superior to those of graphene. So far, only very few MX_2 compounds have been synthesized as suspended single layers, and some of them have been exfoliated as thin sheets. Using first-principles structure optimization and phonon calculations based on density functional theory, we predict that, out of 88 different combinations of MX_2 compounds, several of them can be stable in free-standing, single-layer honeycomb-like structures. Our analysis of stability was extended to include in-plane stiffness, as well as ab initio, finite-temperature molecular dynamics calculations. Some of these single-layer structures are direct- or indirect-band-gap semiconductors, only one compound is half-metal, and the rest are either ferromagnetic or nonmagnetic metals. Because of their surface polarity, band gap, high in-plane stiffness, and suitability for functionalization by adatoms or vacancies, these single-layer structures can be utilized in a wide range of technological applications, especially as nanoscale coatings for surfaces contributing crucial functionalities. In particular, the manifold WX_2 heralds exceptional properties promising future nanoscale applications.

Can Ataca
Department of Materials Science and Engineering,
Massachusetts Institute of Technology, Cambridge,
Massachusetts 02139, United States

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