Stable, Single-Layer MX₂ 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 (MX₂) might offer properties superior to those of graphene. So far, only very few MX₂ 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 MX₂ 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 WX₂ heralds exceptional properties promising future nanoscale applications.