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Air Stability of Two-Dimensional Transition Metal Dichalcogenides[1] SANTOSH KC, ROBERTO LONGO, RAFIK ADDOU, Univ of Texas, Dallas, DIEGO BARRERA, Univ of Texas, Dallas, Centro de Investigación en Materiales Avanzados, México, JULIA W.P. HSU, ROBERT M. WALLACE, KYEONGJAE CHO, Univ of Texas, Dallas — Layered transition metal dichalcogenides (TMDs) have emerged as a potential alternative channel material for ultra-thin and low power nanoelectronics. Highly tunable and unique electronic properties of TMDs made them promising novel materials for various other applications as well. However, in order to realize the superior performance of TMD based devices, the physical and chemical properties need to be understood, in particular their stability under different chemical environments. A detailed comparative analysis of the air stability (i.e., oxygen interaction) of different TMDs is still lacking. We have examined various TMD stabilities in air and found them different from graphene which is stable in air. The changes in the electronic properties with air exposure were studied using density functional theory (DFT), Kelvin probe, and photoelectron emission in air. The results reveal that transition metal sulfides are kinetically more stable than selenides in air, but all TMDs are thermodynamically unstable against oxidation. Furthermore, it is shown that TMD surface defects function as facile oxidation sites impacting their air stabilities. These findings provide helpful guidance to controlled exfoliation and device fabrication processes.

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Santosh KC
Univ of Texas, Dallas

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