Two-Dimensional Transition Metal Dichalcogenides for Photodetection and Biosensing

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Abstract : Transition metal dichalcogenides (TMDs) have gained significant attention as two-dimensional (2D) materials due to their intrinsic band gaps and unique properties, which make them ideal candidates for electronic and photonic applications. Unlike graphene, which lacks a band gap, TMDs (MX_2, where M is a transition metal and X is a chalcogen such as sulfur, selenium, or tellurium) exhibit semiconductor behavior and can be exfoliated into monolayers, enhancing their properties. The properties of these materials are investigated using density functional theory, a quantum mechanical computational method to solve Schrodinger equation for many body problems to calculate electron density of the atoms involved on which the energy and properties of a system depend. They show promise for use in photodetectors, biosensors, memory devices, and other technologies in communications, health, and energy sectors. In particular, metallic TMDs, which lack an intrinsic band gap, benefit from doping with transition metals, this improves their electronic and optical properties. Doping monolayer TMDs yields more significant improvements than doping bulk materials. Notably, doping with metals such as vanadium enhances the magnetization of TMDs, expanding their potential applications in spintronics. This work highlights the effects of doping on TMDs and explores strategies for optimizing their performance for advanced technological applications.

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