Chemistry of TMDs: Distinct Behaviors in Seemingly Similar Materials

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Two-dimensional (2D) materials have become a premier platform for uncovering novel quantum phenomena. The discovery of graphene demonstrated how reduced dimensionality can produce physical behaviors strikingly different from those of bulk systems, while van der Waals (vdW) heterostructures further expand these possibilities. This paradigm shift is driving advances in frontier fields such as spintronics, topological superconductivity, and strongly correlated systems.

Among 2D materials, transition metal dichalcogenides (TMDs) stand out as particularly promising due to their favorable electronic and optical properties combined with exceptional tunability. Yet, despite dominating much of the research landscape, our understanding of this family remains limited—often reduced to broad categorizations of metallic versus semiconducting character, or to quantitative macroscopic properties such as band gap size and carrier mobility.

In reality, TMDs exhibit far greater diversity than these simplified descriptors suggest. Despite their broadly similar crystal structures, transition-metal coordination, and chalcogen valence configurations, subtle structure–property relationships underpin significant differences in their intrinsic physicochemical behaviors. These include variations across pristine monolayers [1–3], the influence of defects such as vacancies [4] and dopants [5–7], and dynamic processes like intercalation [8, 9], all of which collectively define their unique functionalities.

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