Electronic/Optoelectronic Property Tuning in Two-Dimensional Transition Metal Dichalcogenides via High Pressure

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Abstract : The tuneable interlayer interactions in two-dimensional (2D) transition metal dichlcogenides (TMDs) offer an exciting platform for exploring new physics and applications by material variety, thickness, stacking sequence, electromagnetic filed, and stress/strain. Compared with the five methods mentioned above, high pressure is a clean and powerful tool to induce dramatic changes in lattice parameters and physical properties for 2D TMD materials. For instance, high pressure can strengthen the van der Waals interactions along c-axis and shorten the covalent bonds in atomic plane, leading to the typical first-order structural transition (2Hc to 2Ha for MoS2), or metallization. In particular, in the case of WTe_2, its unique symmetry endows the significant anisotropy and the corresponding unexpected properties including the giant magnetoresistance, pressure-induced superconductivity and Weyl semimetal states. Upon increasing pressure, the Raman peaks for WTe_2 at ~120 cm^{-1}, are gradually red-shifted and totally suppressed above 10 GPa, attributed to the possible structural instability of orthorhombic Td phase under high pressure and phase transition to a new monoclinic T' phase with inversion symmetry. Distinct electronic structures near Fermi level between the Td and T' phases may pave a feasible way to achieve the Weyl state tuning in one material without doping.

Keywords : 2D TMDs, electronic property, high pressure, first-principles calculations
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