Quasiparticle energy and band offsets of monolayer of molybdenum and tungsten chalcogenides

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We employ the first-principles single-shot G_0W_0 approach to calculate the quasiparticle energy of monolayer of molybdenum and tungsten dichalcogenides, MX_2 (M=Mo, W; X=S, Se, Te). Beyond calculating bandgaps, we manage to achieve converged absolute band energies relative to the vacuum level. Compared with the results from density functional theory and hybrid functional theory, enhanced many-electron interactions result in substantially larger bandgaps and different absolute band energies. Interestingly, our fully-converged quasiparticle energies ratify the band-gap-center approximation, making it a convenient way to estimate the band offsets of monolayer dichalcogenides. The absolute band energies and corresponding band offsets obtained in this work are important for designing heterojunction devices and chemical catalysts based on monolayer dichalcogenides.