Evolution of the electronic structure of transition metal dichalcogenides with thickness

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The transition metal dichalcogenides exhibit a crossover from a direct band gap semiconductor to an indirect band gap one as the number of layers is increased[1] as well as with strain [2]. The former has been attributed to quantum confinement effects [3], interlayer interactions [4], a combination of both effects [5],and the symmetry of the lattice [6]. I will present our recent results [7] where we have explored a mapping onto a tight binding model to quantify the evolution of the electronic structure as a function of the number of layers. Quantum confinement effects could affect the onsite energies of the orbitals extended into vacuum/van der Waal's gap region as against those orbitals that lie in-plane. Additionally there is a geometric component to it depending on the number of neighbors. Our mapping onto a tight binding model allows us to separate out various contributions to the electronic structure evolution as more layers are added. We find that the onsite energies are almost unchanged as one goes from monolayer to bilayer, indicating that there is no renormalization of onsite energies of orbitals extended into the vacuum region. The evolution of the electronic structure is determined solely by considering interlayer interactions and the geometric part of quantum confinement effects is a part of this. It is indeed surprising that interlayer interactions are important even in these materials which are believed to be van der Waal's heterostructures.

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