

to the tight-binding (TB) description of TMDCs [26, 32, 33, 34, 35, 36, 37, 38], but this approach suffers from the large number of atomic orbitals that have to be included on each site and the need for beyond-nearest-neighbour hopping to account for the variation of the weight of individual atomic orbitals in the band wave functions across the BZ, as revealed by detailed density functional theory (DFT) modelling (see, e.g., Figure 3). The accumulation of experimental data and the drive towards the implementation of monolayer TMDCs in practical devices call for theoretical models of their electronic properties that are both detailed and compact, containing a limited number of parameters while still offering an accurate description.

In this Review, we describe two complementary theoretical approaches that have recently been used to achieve a detailed description of the electronic properties of these materials. One consists of *ab initio* DFT modelling of the band structure, which has the potential to be accurate. DFT can be combined with transport codes [17, 38, 39, 40, 41, 42, 43, 44] or used to calculate optical spectra [45, 46, 47, 48], but *ab initio* calculations are prohibitively expensive for many practical problems focused on modelling devices and studies of, e.g., quantum dots [49, 50]. Moreover, magnetic-field effects [32, 49, 51, 52, 53, 54] and certain questions regarding neutral and charged excitons [55] cannot easily be addressed by DFT-based techniques. The second approach uses the $\mathbf{k} \cdot \mathbf{p}$ methodology [56, 57, 58, 59], which exploits the symmetries of the system. This approach provides an accurate characterisation of the dispersion of the valence and conduction bands in the vicinity of, e.g., the K and $-K$ points and other points of interest in the BZ in terms of a relatively small number of parameters [60]. Magnetic-field and spin-orbit coupling effects can also be taken into account in a straightforward way [49]. In contrast to DFT modelling, this method is only valid in the vicinity of certain high-symmetry \mathbf{k} -space points; however, for those intervals, it enables one to quantify all the essential features of the electronic properties. One can also relate a $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian to a particular TB model [26, 32, 34], although it is not necessary to set up a TB model in order to derive a $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian. Here we present phenomenological $\mathbf{k} \cdot \mathbf{p}$ Hamiltonians derived for all extrema of the bands (at the K , Q , Γ , and M points of the BZ) using the symmetry properties of TMDC atomic crystals, with specific material parameters obtained by fitting them to the DFT band structures of MoS_2 , MoSe_2 , MoTe_2 , WS_2 , WSe_2 and WTe_2 . ‡ The DFT calculations discussed in this Review were

‡ Most of the recent theoretical and experimental work has focused on the properties of MoS_2 , MoSe_2 , WS_2 and WSe_2 , while MoTe_2 and WTe_2 have received much less attention. Bulk MoTe_2 with a trigonal prismatic coordination of the chalcogen atoms (see Figure 1(a)) exists below 815°C (known as α - MoTe_2), whereas above 900°C the crystal structure is monoclinic and the material becomes metallic (β - MoTe_2) [61, 62]. Monolayer samples using liquid exfoliation technique have been obtained from α - MoTe_2 [63], and the optical properties of monolayer [192] the transport properties of few-layer α - MoTe_2 [64, 191] have been investigated recently, giving a clear motivation to include this material in our review. Bulk WTe_2 has an orthorhombic crystal structure, where eight tellurium atoms surround the tungsten atom in a distorted octahedral coordination [65, 66]. Nevertheless, one would expect that it may be possible to grow monolayer WTe_2 with hexagonal prismatic coordination on a suitable substrate. For completeness, therefore, we include this material as well, assuming that its hexagonal