Multiscale investigation of the transport properties in partially overlapped van der Waal structure of 2D materials

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Understanding transport across the vertical stacking of two-dimensional (2D) materials, i.e. in van der Waals homo- and heterostructures, is of primary interest both from a fundamental and from an application-oriented point of view [1]. We present a multiscale method able to compute transport in partially overlapped structures of 2D flakes in a precise and scalable way. Starting from an *ab-initio* DFT [2] calculation of a bilayer (Fig. 1a), we extract a tight-binding-like Hamiltonian expressed in terms of Maximally Localized Wannier Functions [3]. By properly performing the wannierization, it is possible to obtain a bilayer tight-binding Hamiltonian, composed by the specific blocks corresponding to the single layer as in Fig. 1b, in a similar procedure to Refs. [4], which is further exploited to compute transport using the *in-house* software NanoTCAD_ViDES [5], through non-equilibrium Green's function formalism (Fig. 1d). We apply this approach to two different homostructures of MoS_2 and WSe_2, and one heterostructure of MoS_2-WSe_2, considering two different stacking (AA' and AB) (Fig. 2) and several overlaps (from 12 nm up to 100nm). We first exemplify our procedure comparing the bands extracted from the bilayer Hamiltonians of MoS_2 and WSe_2 with the ones obtained from an isolated monolayer (Figs. 3 and 5), evidencing that both the homo- and the heterostructure bilayer Hamiltonians contain the information of the individual layers. Homostructures transmission coefficient are reported in Fig. 4: large differences between the two stacking are observed, while no difference is noticed as the overlapping length is varied (Fig. 4). For the MoS_2-WSe_2 heterostructure, we do not observe any significant variation on the stacking and the overlapping length (Fig. 6), while the null transmission region is widened by the particular alignment of the two materials. The present scheme can be used to study transport in van der Waals devices as well as to understand and investigate transport in highly heterogeneous structures, as the case for 2D inkjet-printed devices [6].

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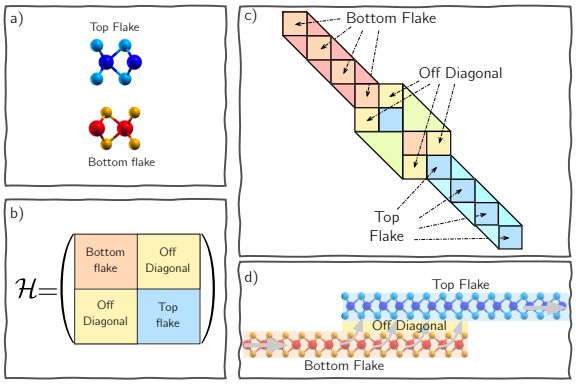

Fig.1: a) Typical simulated structure by ab-initio DFT calculations. b) Schematic depiction of the Wannier Hamiltonian with different blocks indicating, bottom flake (upper left), top flake (bottom right) and the off diagonal elements connecting the two flakes (bottom left and upper right). c) Extended Hamiltonian with different regions of monolayers and overlapping regions (the triangular regions indicate the connections between adjacent cells). d) Schematic depiction of the structure through which transport is computed.

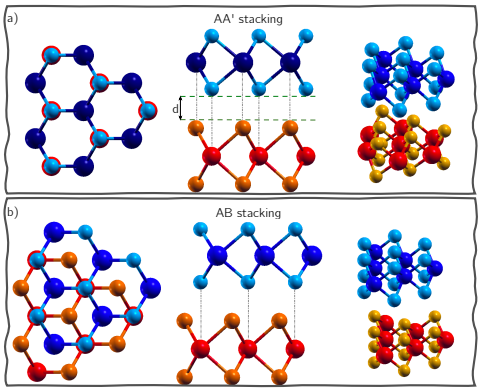

Fig.2: Different TMDs stacking considered a) AA' and b) AB.

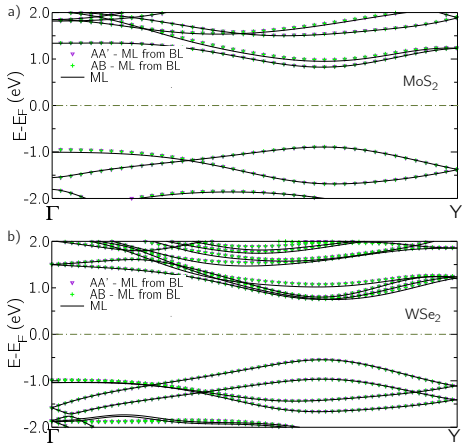

Fig.3: Comparison between monolayer bands (solid line) and extracted bands from bilayer Hamiltonian for a) MoS_2 and b) WSe_2 for the different stacking considered.

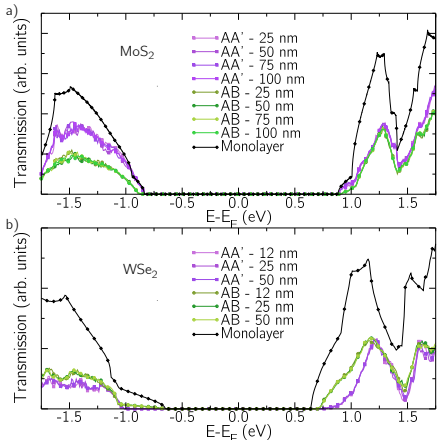

Fig.4: Transmission coefficient for a) MoS_2 and b) WSe_2 for the two different stacking considered and for overlapping length ranging from 12 nm till 100 nm. For comparison the monolayer transmission is reported for both materials.

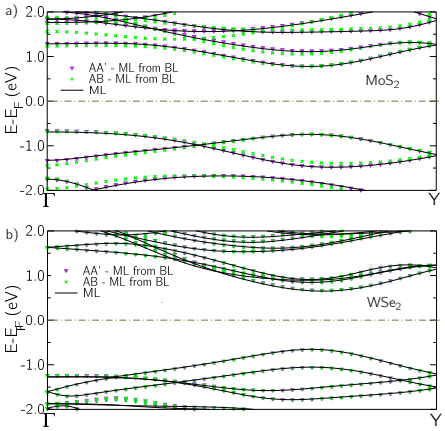

Fig.5: Comparison between monolayer bands (solid line) and extracted bands from the heterostructure bilayer Hamiltonian for a) MoS_2 and b) WSe_2 for the different stacking considered.

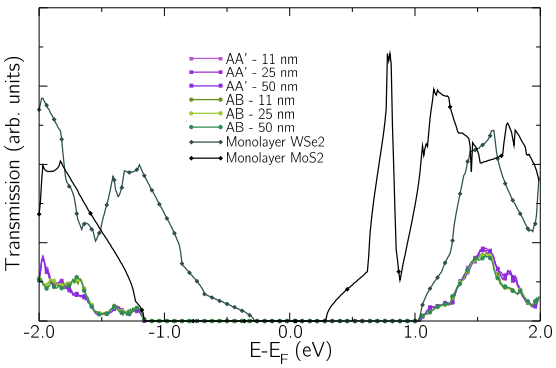

Fig.6: Transmission coefficient for the MoS_2-WSe_2 heterostructure for different overlapping lengths for the two stackings considered. Monolayer of isolated MoS_2 and WSe_2 are reported for reference.

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