Large scale calculations of electronic structure of 2D Crystals

J. L. Lado and J. Fernandez-Rossier

International Iberian Nanotechnology Laboratory, Braga (Portugal)
jose.luis.lado@gmail.com

Abstract

Numerical studies of electronic properties often have to trade off accuracy by computation time. Thus, density functional theory (DFT) methods are known to deal accurately with ground state properties of many materials, but become impractical, or even impossible, when it comes to describe nanostructures with thousands of atoms. In those instances, it becomes convenient to use tight-binding models, but these are some times inaccurate, or worse, unavailable.

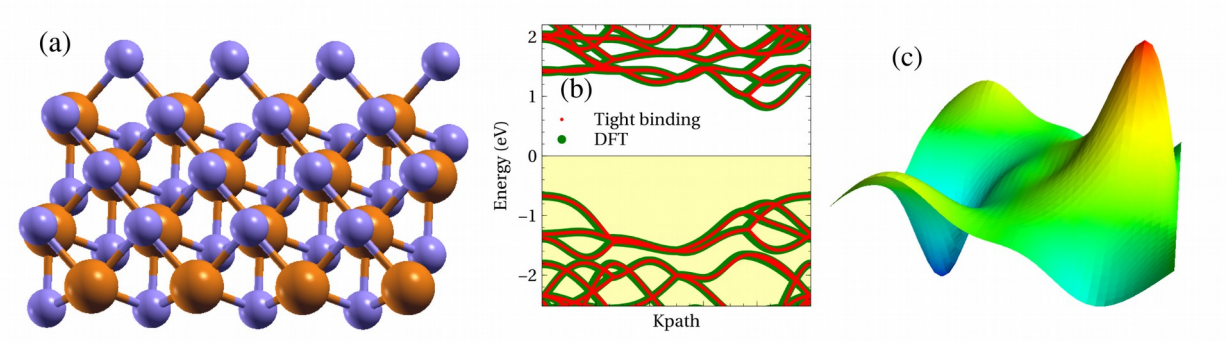
Here we try to go around this trade-off building tight-binding models derived from DFT calculations using the well known Wannierization method [1]. We apply this approach to a variety of 2D crystals, such as MoS_2, black phosphorous and graphene, and we use it to calculate Landau Levels and edge states in a stripe geometry. Combined with Kernel Polynomial method [2], this approach permits to calculate the energy levels of 2D flakes of up to 10000 atoms in a conventional laptop, starting from accurate DFT Hamiltonians. Both the potential and the shortcomings of this approach will be discussed during the talk.

References

[1] Nicola Marzari, Arash A. Mostofi, Jonathan R. Yates, Ivo Souza, and David Vanderbilt, Rev. Mod. Phys. 84, 1419 (2012)

[2] Alexander Weiße, Gerhard Wellein, Andreas Alvermann, and Holger Fehske, Rev. Mod. Phys. 78, 275 (2006)

Figures



Example of the multiscale approach described above, applied to the chalcogenide MoS_2 whose structure is shown in (a). First, ab-initio electronic structure calculations are performed, then Wannierization is carried out, yielding a real space tight binding Hamiltonian. A comparison of the band structure for a 2x2 supercell of MoS_2 is shown in (b), proving an excellent agreement between the DFT and Wannier band structures. The tight binding Hamiltonian will allow to calculate conventional electronic properties of the system, analyzing the effect of disorder or studying Quantum Hall effect. In particular, we show in (c) the Berry curvature in the 2d Brillouin zone, were it can be observed that a large anomalous velocity arises in the folded K and K' valleys.