Layered and 2D materials: electronic properties and structural instabilities from first principles

Pablo Ordejón[1]
B. Guster[1], M. Pruneda[1], E. Canadell[2]

[1]*Catalan Institute of Nanoscience and Nanotechnology – ICN2, CSIC and BIST, 08193 Bellaterra, Barcelona (Spain)*

[2]*Institut de Ciència de Materials de Barcelona, CSIC, 08193 Bellaterra, Barcelona (Spain)*

pablo.ordejon@icn2.cat

I will present some of our recent work [1-3] on the understanding of the electronic properties of layered materials and their 2D relatives by means of first principles electronic structure calculations. In particular, I will focus on the correlation between the crystal structure and the electronic properties, with special emphasis on the structural instabilities with an electronic origin. This will be done in connection with recent experimental studies that have been able to demonstrate the presence of charge density waves (CDW) in several 2D single-layer materials like $NbSe_2$ and $TiSe_2$. The evolution of the CDW with external electrostatic doping, which has been achieved experimentally using field effect transistor setups, will be analysed for the case of $TiSe_2$ [4].

Figures

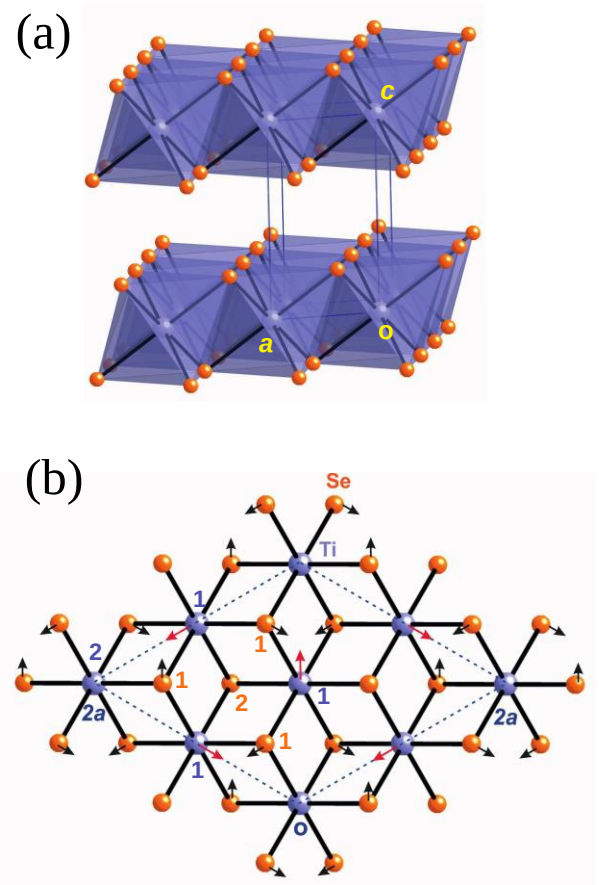

Figure 1: (a) Crystal structure of $TiSe_2$. (b) Schematic representation of the displacements occurring in a single-layer of the 2x2 CDW structure of $TiSe_2$.

References

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