Spatial prediction and evolution of molecular orbitals in 2D-materials crystals by Machine Learning

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Abstract

The electronic characteristics for 2D nanostructures, such as graphene and layered transition metals dichalcogenides, pose great advantages for the semiconductor and advanced electronics industries. Currently, the determination of these characteristics is carried out by standard computational methods such as Density Functional Theory (DFT), which are high-demanding in terms of computational resources and time. New approaches, based on artificial intelligence methods such as Machine Learning (ML), have demonstrated high potential as alternatives for the efficient determination of physical and electronic characteristics of materials and nanostructures, in terms of computing time and power [1-3]. This talk describes further investigations on the use of ML algorithms for the prediction of STM images, and the spatial determination of molecular orbitals along high symmetry points within crystalline cells of 2D layered nanostructures. In specific, the spatial characteristics of the highest-occupied-molecular-orbital (HOMO) and lowest-unoccupied-molecular-orbital (LUMO) for pristine and doped graphene, and MoS_2, are addressed. These results contribute to the discussion on the impact and potential applications of ML methodologies on the computational nanotechnology research.

References

[1] Zeliang Liu, Chengtang Wu, Masataka Koishi, Computer Methods in Applied Mechanics and Engineering, 345 (2019) 1138.
[2] Ashwin Mhadeshwar, Trupti Mohanty, Taylor D. Sparks, Journal of Materials Informatics, 4 (2024) 12.
[3] Rubén Guerrero-Rivera, Francisco J Godínez-García, Takuya Hayashi, Zhipeng Wang, Josué Ortiz-Medina, Computational Materials Science, 242 (2024) 113076.

Figures

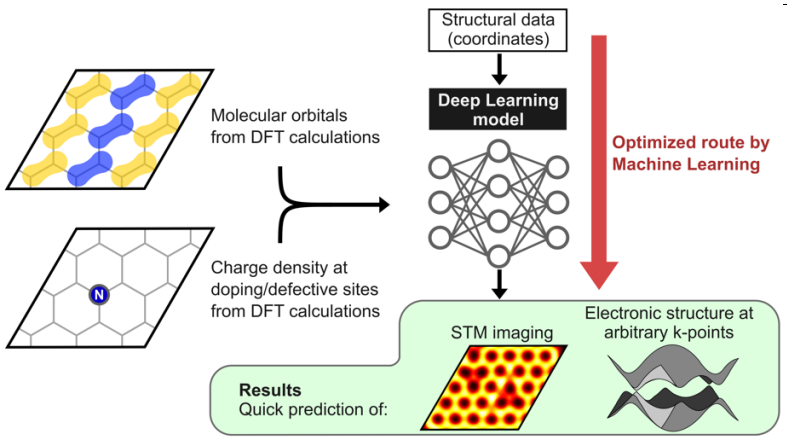

Figure 1: Scheme of the optimized method for prediction of graphene STM images and electronic structure at arbitrary *k*-points, by means of a deep-learning model trained on molecular orbitals and localized charge density, obtained by DFT calculations.