Some recent advances in 2D materials and surface science seen through ab initio calculations

S. LEBEGUE,
LPCT, CNRS and Université de Lorraine
E-mail : sebastien.lebegue@univ-lorraine.fr

Abstract:
In the field of nanosciences, research on materials has made spectacular progress over the last twenty years. In this talk, I will present, through some examples from recent works, how ab initio calculations can provide a better understanding of the physical and chemical properties of different compounds. In particular, I will discuss our recent works [1,2, 3] on the properties of indium and gallium chalcogenides 2D systems interfaced with other bidimensional systems such as graphene, blue-phosphorene, or Bi2Se3. Then I will present our recent results [4] concerning the electronic structure of systems consisting of different halogen atoms adsorbed on Cu (111) and Cu (110) surfaces. Our results are compared with ARPES and STS experiments and an excellent agreement between theory and experiment was found. Finally, some current limits as well as future challenges for ab initio calculations will be described briefly.

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[2] T. Ayadi, L. Debbichi, M. Badawi, M. Said, D. Rocca, S. Lebègue, Applied Surface Science, 538, 148066 (2021)
[3] T. Ayadi, M. Badawi, M. Said, and S. Lebègue, Physica E, 115115, 139 (2022)
[4] Won June Kim, Sarah Xing, Geoffroy Kremer, Muriel Sicot, Bertrand Kierren, Daniel Malterre, Giorgio Contini, Julien Rault, Patrick Le Fèvre, Francois Bertran, Dario Rocca, Yannick Fagot-Revurat, and Sébastien Lebègue, J. Phys. Chem. C. 123, 26309-26314 (2019)