Labex MATISSE

Axe 4

"Theoretical modeling of electrochemically-doped superconducting nanolayers"

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Hosting laboratories, teams and and thesis supervisors names:

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Research project

We developed a first-principles theoretical approach to field-effect doping and the method was implemented in the QuantumEspresso package. The method allows for calculation of the electronic structure as well as complete structural relaxation in field-effect configuration using density-functional theory. Up to now, this was computationally expensive and in some case even impossible. Thus, experimentalists were forced to use simplified screening models in order to determine the induced charge from Hall-effect measurements. Yet, it is unknown to what extend this simple models hold in nanolayers systems and what are the changes which are induced by the large local electric fields (in the order of 1 V/nm).

Scientific results & impacts

We described the field-effect doping of nanolayers such as ZrNCl or transition-metal dichalgonides (TMDs). We have shown that, *e.g.*, only one ZrNCl layer is doped and that this induces large structural changes. In TMDs we found only small structural changes. Yet, the correct modeling of the asymmetric electric field proved to be essential. Further-more, we have shown that Hall measurements can overestimate the induced charged.

Main key facts

Publications :

- Electrochemical doping of few-layer ZrNCl from first principles: Electronic and structural properties in field-effect configuration, T. Brumme, M. Calandra, and F. Mauri, Phys. Rev. B 89, 245406 (2014)
- First-principle theory of field-effect doping in transition-metal dichalcogenides: Structural properties, electronic structure, Hall coefficient, and electrical conductivity, T. Brumme, M. Calandra, and F. Mauri, accepted for publication in PRB
- Evidence for Flat bands near Fermi Level in Epitaxial rhombohedral Multilayer Graphene, D. Pierucci, H. Sediri, M. Hajlaoui, J.-C. Girard, T. Brumme, M. Calandra, E. Velez-Fort, G. Patriarche, M. G. Silly, G. Ferro, V. Soulière, M. Marangolo, F. Sirotti, F. Mauri and A. Ouerghi, accepted for publication in ACS Nano