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'Electronic structure and charge transport simulations in GRM-organic hybrids: Where Chemistry meets Physics'

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Abstract
The electronic structure of 2D materials can be profoundly affected by physical or chemical adsorption of (electro-active) conjugated molecules. The presence of adlayers manifests as changes in the work function and electrical doping and can be used to tune charge carrier mobility and conductivity. In this talk, we will review recent first-principles simulations performed in our group to model:

(i) The doping of monolayer transition metal dichalcogenies via physisorption of aromatic solvent molecules [1].
(ii) The control of charge carrier density in superlattices formed by photochromic molecules self-assembled on graphene [2].
(iii) The engineering and healing of chemically active defects in monolayer MoS2 [3].
(iv) The charge transport in photoswitchable self-assembled monolayers organic-graphene hybrids [4].

References

[1] Y. Wang et al. J. Phys. Chem. Lett. 10 (2019) 540-547.
[2] M. Gobbi et al. Nature Communications 9 (2018) 2661.
[3] S. Bertolazzi et al. Advanced Materials 29 (2017) 1606760.
[4] C. Tonnelé et al., JPhysMaterials, in press.

Figures

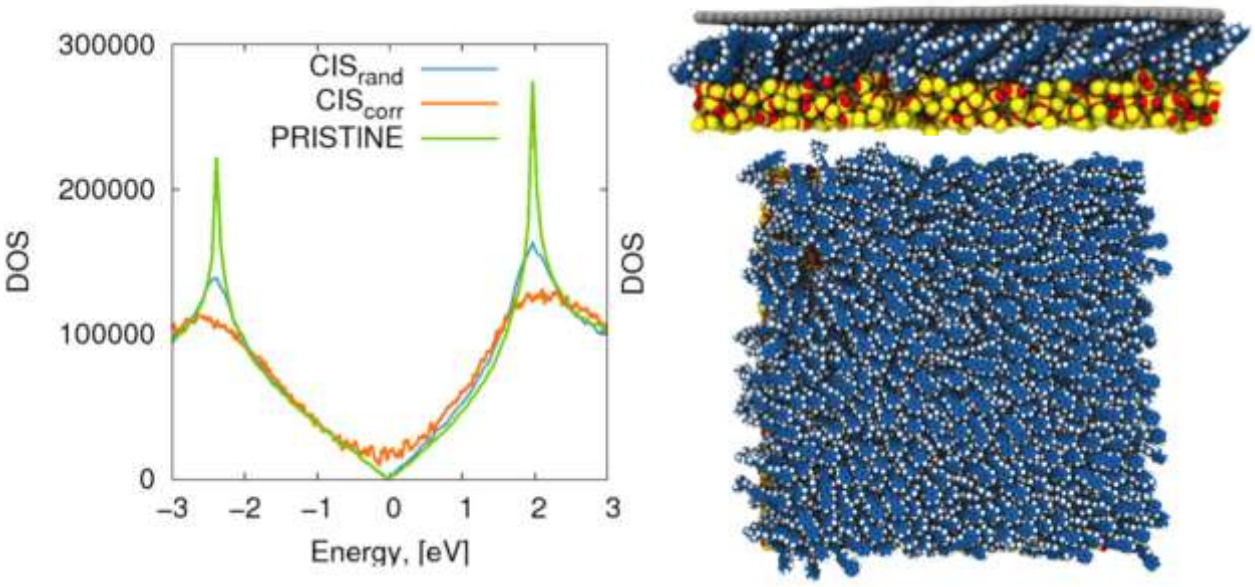

Figure 1: (right) Side and top views of a graphene layer deposited on a SAM-decorated silica surface. (left) DOS of the pristine graphene and in presence of an underlying SAM-on-silica with the photochromic molecules in the CIS form. Adapted from Ref. 4.