When graphene meets perovskites

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Abstract
In recent years the energy conversion efficiency of solar cells based on halide perovskites skyrocketed above 20%, making these systems among the most promising solution-processable photovoltaics technology to date. At the same time graphene is the prime candidate for TCO replacement in optoelectronic devices. Given the exceptional and complementary properties of these two materials, it is expected that their combination into the same device may lead to significant improvements in solar energy technology and light-emitting devices. During the past three years in our group at Oxford we have been investigating photovoltaics materials based on graphene, perovskites, and their combinations using state-of-the-art atomic-scale first-principles calculations [1-7]. In the first part of the talk I will describe our work on graphene/perovskite composites [1]. Unexpectedly we found that even for ideal planar interfaces between graphene and perovskites, the interface chemistry induces an unusual ferroelectric distortion in the perovskite layer, which results from a slight octahedral tilt in the basal plane (Figure 1). Our calculations show that this interfacial ferroelectricity should carry the dual advantage of promoting charge extraction and inhibiting electron-hole recombination. If confirmed by experiments, this mechanism could not only be important in photovoltaics, but also provide new pathways for engineering ferroelectricity in other graphene/perovskite interfaces, for example in the context of solar water splitting. In the second part of the talk I will discuss our recent work in the area of computational modelling of graphene/polymer interfaces for organic solar cells, as well as high-throughput computational searches for Pb-free photovoltaic perovskites. In the former case we investigated the role of functional groups on the interfacial energy-level alignment and on the photovoltage [3]. In the latter case we performed a computational screening of all hypothetical halide perovskites with divalent metal cations, and identified Mg as a candidate for partial Pb replacement [7].

References

[1] G. Volonakis, F. Giustino, J. Phys. Chem. Lett., **6** (2015) 2496.
[2] M. R. Filip, G. E. Eperon, H. J. Snaith, F. Giustino, Nat. Commun., **5** (2014) 5757.
[3] K. Noori, D. Konios, M. Stylianakis, E. Kymakis, F. Giustino, 2D Mater., **3** (2016) 015003.
[4] M. R. Filip, F. Giustino, Phys. Rev. B, **90** (2014) 245145.
[5] M. R. Filip, C. Verdi, F. Giustino, J. Phys. Chem. C, **119** (2015) 25209.
[6] M. A. Perez-Osorio, R. L. Milot, M. R. Filip, J. B. Patel, L. M. Herz, M. B. Johnston, F. Giustino, J. Phys. Chem. C, **119** (2015) 25703.
[7] M. R. Filip, F. Giustino, J. Phys. Chem. C, **120** (2016) 166.

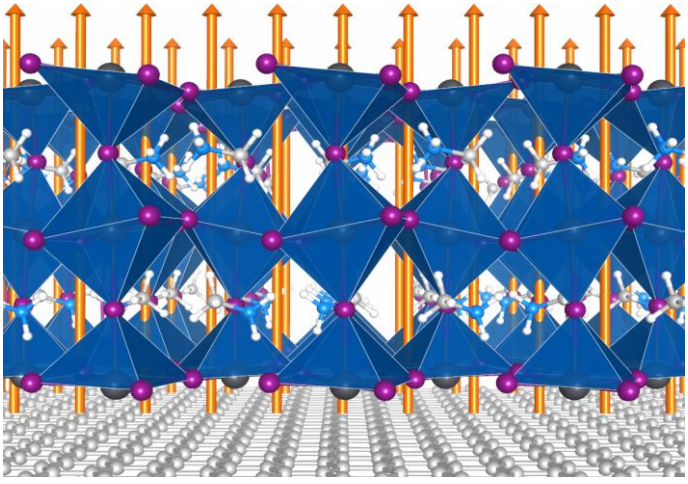

Figure 1 Induced ferroelectricity at the interface between graphene and the halide perovskite MAPbI3.