THE ENERGY LEVELS IN HOLE-DOPED MOLECULAR SEMICONDUCTORS

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Understanding the nature of charge carriers in organic thin films is crucial in order to achieve rational design in opto-electronic organic devices. In the present work, we rely on interface doping phenomena, as occurring when contacting an organic semiconductor with a high work function (modified) electrode, to study the electronic properties of a hole-doped molecular thin film [1,2]. The investigated system, consisting of a C_{60} film adsorbed Au(111) pre-covered with a thin MoO_3 layer, is studied by direct and inverse photoemission. A detailed analysis of the photoemission spectra, supported by theoretical calculations based on density functional theory, helps to precisely identify the corresponding density of states of the neutral and positively charged C_{60} coexisting at the surface.

The obtained results reveal a picture of the electronic structure which strongly differs from the traditionally conceived one, i.e. with the energy levels consisting of singly occupied molecular states lying within the energy gap of the semiconductor (Fig. 1. a) [3]. Instead, here we demonstrate that the on-site Coulomb repulsion splits the partially unoccupied frontier molecular level in the p-doped systems into two sub-levels (Fig. 1. b) [1]. The role of inter-site Coulomb interaction between molecular ions and neighbor molecules is further addressed and allows providing a complete picture of the energy levels of molecular semiconductors in the presence of excess charges [1].

Keywords: Organic semiconductors; photoemission; electronic structure; hole-doping

References

[1] S. Winkler, P. Amsalem, J. Frisch, M. Oehzelt, G. Heimel, N. Koch, Materials Horizons 2 (2015) 427.
[2] M. Oehzelt, N. Koch and G. Heimel, Nat. Commun. 5 (2014), 4174.
[3] J. L. Bredas and G. B. Street, Acc. Chem. Res. 18 (1985) 309.

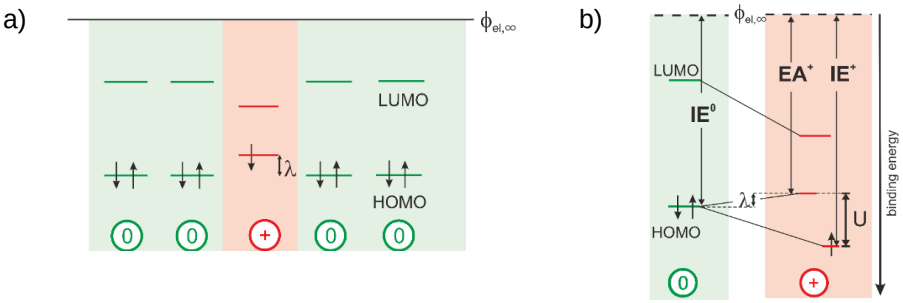

Fig. 1. a) Traditionally envisioned energy levels of positive polarons (red) embedded in a neutral organic matrix (green). b) Effect of the on-site Coulomb repulsion on the frontier energy levels upon hole doping as determined by (inverse) photoemisson.