Molecular systems in complex environments: an embedded many-body perspective

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Molecules between two metallic electrodes, at a donor/acceptor interface, in a solvent or a biological environment, are few examples of systems associated with different properties and applications. They share however a common characteristic, namely they are active sub-systems immersed in a complex and large, often disordered, environment that strongly renormalizes their electronic properties (energy levels, optical spectra, conductance, etc.) We will present a specific family of *ab initio* techniques, namely embedded many-body perturbation theories [1,2] allowing to study the electronic and optical excitations of active subsystems immersed in very large scale electrostatic and dielectric media. The case of molecular dopants [3] and defects in stacked 2D materials [4] will be given as important examples of the usefulness of such theoretical approaches. Work done in collaboration with G. D'Avino, J. Li, D. Amblard, M. Comin, S. Fratini (Institut Néel, Grenoble), I. Duchemin (CEA, Grenoble), D. Beljonne (Mons, Belgium) and D. Jacquemin (Univ. Nantes).

References

[1] Li, D'Avino, Beljonne, Duchemin, Blase, J. Phys. Chem. Lett. **7** (2016) 2814.
[2] Blase, Duchemin, Jacquemin, Chem. Soc. Rev. **47** (2018) 1022.
[3] Comin, Fratini, Blase, D'Avino, Adv. Mater. **34** (2022) 2105376.
[4] Amblard, D'Avino, Duchemin, Blase, Phys. Rev. Mater. **6** (2022) 064008.

Figures

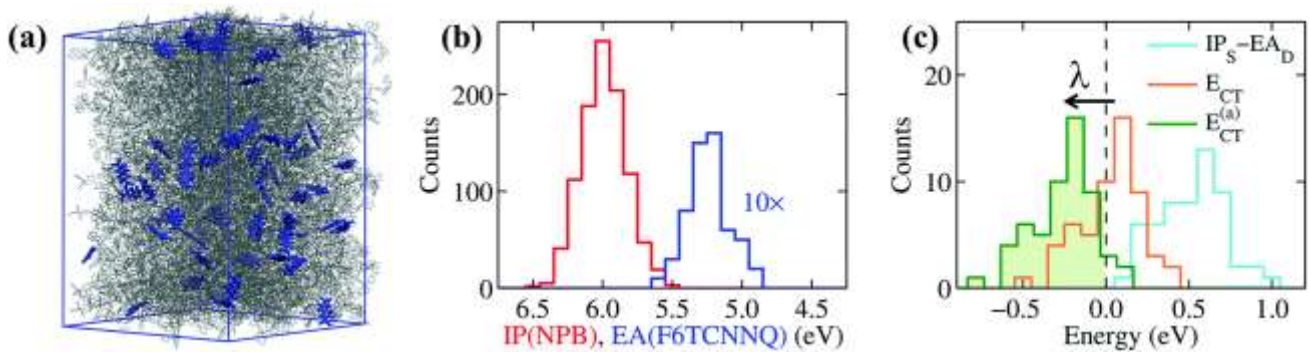

Figure 1: (a) Doped amorphous organic semiconductor with dopants (acceptors) in blue. In (b) Distribution of host highest occupied (red) and dopant acceptor (blue) levels within accurate embedded many-body *GW* calculations. c) Histogram of charge-transfer excitation energies from dopants to host with polaronic contribution (λ). From Li *et al.* Mater. Horizons, **6** (2019) 107.