THEOS
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Modeling dye-sensitized and perovskite solar cells from first principles: challenges and perspectives

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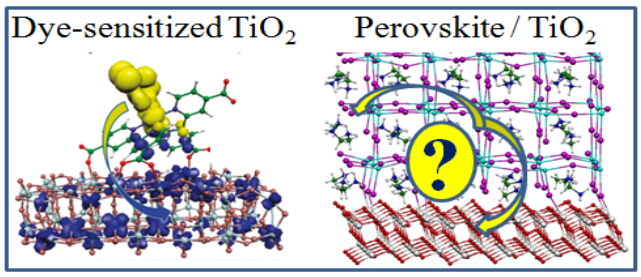
Abstract: Over the last two decades, researchers have invested enormous efforts into hybrid/organic photovoltaics, leading to the recent launch of the first commercial products that use this technology. To effectively compete with conventional photovoltaics, emerging technologies such as dye-sensitized solar cells (DSCs), need to achieve higher efficiency and stability, while maintaining low production costs. Organohalide lead-perovskites have revolutionized the hybrid/organic photovoltaics landscape. Despite the fast increase of efficiency, currently topping at 22%, some of the materials properties related to their extraordinary photovoltaic performance remain largely not understood. Further advances in the perovskite solar cells (PSCs) field may be boosted by computational design and screening of new materials, with researchers examining material characteristics that can improve device performance and/or stability. Suitable modeling strategies may allow researchers to observe the otherwise inaccessible but crucial hetero-interfaces that control the operation of both DSCs and PSCs, allowing researchers the opportunity to develop new and more efficient materials and optimize processes.



In this talk, I will illustrate the performance of an integrated simulation toolbox, rooted into Density Functional Theory, ab-initio molecular dynamics and many body GW methods including spin-orbit coupling, that can provide atomistic electronic structure information on the materials properties and on the crucial dye or perovskite absorbers/metal-oxide/hole transporter material heterointerfaces. The accuracy of various computational approaches is critically assessed against related experimental data and the representative interfaces that control the device operational mechanism are analyzed. In particular, the focus is posed on the structural and electronic features of the dyes and perovskites interfaces with various metal oxide substrates, i.e. TiO_2, Al_2O_3 and ZnO, with emphasis on electronic interfacial and dynamical properties. The role of defects and their migration at the $MAPbI_3$ / TiO_2 interface are also discussed. The challenges for theory and computation and a perspective of future directions in the field are finally discussed.

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