Modeling devices for photovoltaics : insights from ab-initio approaches

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Abstract

A general overview of ab-initio approaches essentially rooted on Density Functional Theory, for the description of the structural and electronic properties ruling the macroscopic behavior of devices for photovoltaics applications, will be given through selected examples. In particular, this talk will be focused on the computational approaches enabling the description and the design of dye sensitized solar cells (DSSCs) and quantum dot sensitized solar cells (QDSCs) in order to highlight both their success and their current limitations. Examples of the application of these methods -ranging from the modeling of photovoltaic characteristic of DSSCs to the relation between the morphological and the charge transport properties in hole transporter materials for energy devices- will be provided.

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