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Editorial

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Nano-Enabled Photovoltaics. Progress in Materials and Methodologies

Nanoenabled photovoltaics consist of a family of related approaches to make solar cells that use nanosized material elements, involving a combination of inorganic and organic components and hard and soft matter, including liquid electrolytes, which are combined using low-cost preparation methods, mainly by low-temperature solution processes. This type of solar cells have been developed rather strongly in recent times in three main directions, dye-sensitized solar cells (DSCs), organic bulk heterojunction solar cells (BHJs), and quantum dot (QD)-based solar cells. The progress has been realized in new molecules, materials, and preparation methods that boosted the performance in many of these types of solar cells. On another hand, a wide range of scientific work involving characterization tools and modeling has produced detailed understanding of many features of the device operation. The Perspectives presented in this issue show an updated view of these aspects of development of the nanostructured solar cells.

At the core of the operation of a DSC is the junction of the TiO_2/dye/hole conductor where charge photogeneration and separation are realized. It has also been recognized that molecular dye properties and coabsorbents play a central role in the rate of recombination of the electrons injected in TiO_2 back to the electrolyte or to the oxidized dye. Due to the combination of effects that control the operation of the junction, it is not easy to obtain experimental information that isolates specific features. Pastore and De Angelis in their Perspective (Pastore, M.; De Angelis, F. Intermolecular Interactions in Dye-Sensitized Solar Cells: A Computational Modeling Perspective. *J. Phys. Chem. Lett.* **2013**, *4*, 956−974) introduce a wide range of computational modeling methods to describe the dye-sensitized interface. In the first part of the review, they summarize knowledge that has been gathered about different interactions of the semiconductor−dye−redox shuttle−coadsorbent system. Thereafter, they use detailed atomistic and molecular modeling methods to treat a range of specific phenomena, such as dye binding, dye aggregation, and cosensitization, all of which have a determinant influence in the operation of high-performance DSC devices. The Perspective of Le Bahers, Adamo, Ciofini, and co-workers, (Le Bahers, T.; Pauporte, T.; Laine, P. P.; Labat, F.; Adamo, C.; Ciofini, I. Modeling Dye-Sensitized Solar Cells: From Theory to Experiment. *J. Phys. Chem. Lett.* **2013**, *4*, 1044−1050) also explores the application of the computational approaches of density functional theory (DFT) and time-dependent DFT to the DSC, focusing on the prediction of the macroscopic observables like the photocurrent and external quantum efficiency based on microscopic and molecular modeling of the semiconductor−dye−hole conductor complex.

The organic BHJ solar cell consists of a blend of donor and acceptor organic materials, which are basically symmetrical from a morphological point of view. The mechanism of operation for the photovoltaic action has been the object of many discussions, and the role of selective contacts, able to take either electrons or holes out to the metal, has been emphasized.[1] The Perspective by Garcia-Belmonte and co-workers (Garcia-Belmonte, G.; Guerrero, A.; Bisquert, J. Elucidating Operating Modes of Bulk-Heterojunction Solar Cells from Impedance Spectroscopy Analysis. *J. Phys. Chem. Lett.* **2013**, *4*, 877−886) summarizes recent understanding of the BHJ applying the method of impedance spectroscopy (IS), that has become already well-established in the DSC area. In this Perspective, the authors bring together a broad set of results that show that different combinations of fullerenes and light-absorbing polymers can be well-understood on the basis of a doped blend that has a significant density of (hole) majority carriers. The stable population of the majority carriers enables the use of a simple model for IS that consists of the chemical capacitance and recombination resistance. This approach provides a great deal of information concerning kinetic and energetic features of the BHJ solar cell, starting from IS data at different voltages.

The QD solar cells have come to the forefront of research in two main configurations, the QD-sensitized solar cell, similar to the DSC but requiring specific tailoring of many device aspects,[2] and solar cells based on lead chalcolgenide colloidal QDs that are solidified into a thin film by organic linkers.[3,4] In addition, very recently, a new class of organometal halide perovskite absorbers was presented, which showed power conversion efficiencies around 10%, with hints of ambipolar transport in the absorber itself, holding great promise for new routes of development of this field.[5,6] These exciting developments lead Kamat to propose in his Perspective that the QD solar cell will be "The Next Big Thing" in photovoltaics, (Kamat, P. V. Quantum Dot Solar Cells. *The Next Big Thing* in Photovoltaics. *J. Phys. Chem. Lett.* **2013**, *4*, 908−918), an idea that is shared by many scientists that have hasted to try a hand in these topics, in prevision of a large development of improved materials, devices, and new operation modes. Kamat presents an overview of the methods of preparation of materials and devices of the different classes of QD solar cells, and he describes as well a range of emerging strategies to improve the solar cell performance, including the multiple exciton generation, application of plasmonic resonance of metal nanoparticles, and several composite concepts of layers and sensitizers to optimize light harvesting.

These Perspectives show that the study of complex combinations of nanomaterials and molecules, in nano-enabled photovoltaics, is providing many advances in the understanding of electronics and photonics at the nanoscale, with a view to strong devices that may make their way to the market.

Juan Bisquert,* Senior Editor

Photovoltaics and Optoelectronic Devices Group, Departament de Física, Universitat Jaume I, 12071 Castelló, Spain

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AUTHOR INFORMATION

Corresponding Author

*E-mail: bisquert@uji.es.

Notes

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