Modeling Materials and Processes in Hybrid/Organic Photovoltaics: From Dye-sensitized to Perovskite Solar Cells

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Over the last two decades, researchers have invested enormous research effort into hybrid/organic photovoltaics, leading to the recent launch of the first commercial products that use this technology. Dye-sensitized solar cells (DSCs) have shown clear advantages over competing technologies. The top certified efficiency of DSCs exceeds 11% and the lab-cell efficiency is greater than 13%.

In 2012, the first reports of high efficiency solid-state solar cells based on organohalide lead perovskites completely revolutionized the field. These materials are used as light-absorbers in DSCs and as light-harvesting and electron conductor in meso-superstructured and flat heterojunction perovskite solar cells (PSCs) and show certified efficiencies that in 2016 exceeded 22%.

To effectively compete with conventional photovoltaics, emerging technologies need to achieve higher efficiency and stability, while maintaining low production costs.

Many of the advances in the DSCs and PSCs field have relied on the computational design and screening of new materials. Suitable modeling strategies further allow researchers to observe the otherwise inaccessible but crucial hetero-interfaces that control the solar cell operation, allowing researchers the opportunity to develop new and more efficient materials and optimize processes.

We illustrate the basic device architectures and operating principles of both DSCs and PSCs highlighting the fundamental modeling strategies and revealing fundamental aspects of the device's operational mechanism. Although the modeling of DSCs is relatively mature, the recent "perovskite storm" has presented new problems and new modeling challenges, such as understanding exciton formation/dissociation at interfaces and carrier recombination in these materials.

References:

1. F. De Angelis *Acc. Chem. Res.* **2014**, 47, 3349.
2. F. De Angelis, C. Di Valentin, S. Fantacci, A. Vittadini, A. Selloni *Chem. Rev.* **2014**, *114*, 9708.
3. Bai, Y.; Mora-Seró, I.; De Angelis, F.; Bisquert, J.; Wang, P. *Chem. Rev.* **2014**, *114*, 10095.Domansk, K.; Roose B.; Matsui, T.; Saliba, M.; Turren-Cruz, S-H.; Correa-Baena, J-P.; Carmona, C. R.; Richardson, G.; J. M., Foster; De Angelis, F.; Ball, J. M.; Petrozza, A.; Mine, N.; Nazeeruddin, M. K.; Tress, W.; Grätzel, M.; Steiner, U.; Anders Hagfeldtd, A.; Abate, A. *Energy Environ. Sci.* **2017**, *10*, 604.
4. Mosconi, E.; Meggiolaro, D.; Snaith, H.; Stranks, S. D.; De Angelis, F. *Energy Environ. Sci.* **2016**, *9*, 3180.
5. Quarti, C.; Mosconi, E.; Ball, J. M.; D'Innocenzo, V.; Tao, C.; Pathak, S.; Snaith, H.; Petrozza, A.; De Angelis, F. *Energy Environ. Sci.* **2016**, *9*, 155.
6. Azpiroz, J. M.; Mosconi, E.; Bisquert, J.; De Angelis, F. *Energy Environ. Sci.* **2015**, *8*, 2118