

[SY-A6] Symposium A-6

Chair: Emma Griffiths (University of Cape Town, South Africa)

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[SY-A6] Multiscale modeling of advanced materials for hybrid organic-inorganic solar cells

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When it comes to talk about alternatives to non-renewable sources of energy, photovoltaics is one of the most promising choices for converting solar light into electricity with the use of solar cells. At present, there is wide variety of solar cell devices on the market and this variety will continue to grow because of the race for better conversion efficiency and the final product sustainability. Within recent years, the seemingly clear boundaries between photovoltaics of inorganic and organic solar cells have started to fade by the advent of metal-halide hybrid organic-inorganic perovskites (OIP). They are very promising candidates for future photovoltaic applications because they have wide-direct band gap, which can be tuned by either changing the organic cation, the metal atom, or the halide. Their power conversion efficiency now reached over 22%. At the same time, the level of our understanding of the origin of such performance is still insufficient. We believe that thin film morphology is a key factor determining the performance of bulk heterojunction organic solar cells, because of its influence on charge separation, charge transport and recombination losses in donor-acceptor blends. With this respect, we present both descriptive and predictive multiscale modeling of electronic and structural properties of blends of PCBM or hybrid OIP of the type $\text{CH}_3\text{NH}_3\text{PbX}_3$ ($\text{X}=\text{Cl}, \text{Br}, \text{I}$) with P3HT, P3BT or squaraine SQ2 dye sensitizer, including adsorption on TiO_2 clusters. Here, the multiscale nature of modeling means that in a set of simple hierarchical approaches we combine different methods for different scales (quantum mechanical, microscopic, mesoscopic) interpreted independently and that the information obtained at one level is transmitted to the next level as a required input. If necessary, new information is sometime transmitted back to the previous level for a feedback control. As the result, we arrive at a very reliable methodology that allows computing the microscopic structure of blends on the nanometer scale and getting insight on miscibility of its components at various thermodynamic conditions. The calculated nanoscale morphologies serve as an instrument in rational design of hybrid OIP. They are used in collaboration with experts who actually make prototypes or devices for practical applications.