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Statistical Mechanical Approach in Modeling of Hybrid Solar Cells for Photovoltaic Applications

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Abstract : We present both descriptive and predictive modeling of structural properties of blends of PCBM or organic-inorganic hybrid perovskites of the type CH3NH3PbX3 (X=Cl, Br, I) with P3HT, P3BT or squaraine SQ2 dye sensitizer, including adsorption on TiO2 clusters having rutile (110) surface. In our study, we use a 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 methodology is based on the integral equation theory of molecular liquids in the reference interaction site representation/model (RISM) and uses the universal force field. Input parameters for RISM, such as optimized molecular geometries and charge distribution of interaction sites, are derived with the use of the density functional theory methods. To compare the diffusivity of the PCBM in binary blends with P3HT and P3BT, respectively, the study is complemented with MD simulation. A very good agreement with experiment and the reports of alternative modeling or simulation is observed for PCBM in P3HT system. The performance of P3BT with perovskites, however, seems as expected. The calculated nanoscale morphologies of blends of P3HT, P3BT or SQ2 with perovskites, including adsorption on TiO2, are all new and serve as an instrument in rational design of organic/hybrid photovoltaics. They are used in collaboration with experts who actually make prototypes or devices for practical applications.

Keywords : multiscale theory and modeling, nanoscale morphology, organic-inorganic halide perovskites, three dimensional distribution
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