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Organic-inorganic hybrid solar cells for photovoltaic applications: Modeling the effect of molecular structure and environment on miscibility and morphology of bulk heterojunctions

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Both descriptive and predictive modeling of structural properties of blends of PCBM or organic-inorganic hybrid perovskites of the type $CH_3NH_3PbX_3$ (X=Cl, Br, I) with P3HT, P3BT or some squaraine SQ dye sensitizer, including adsorption on TiO_2 clusters having rutile (110) surface, is presented with the use of 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 remarkably good agreement with available experimental data and results of alternative modeling/simulation is observed for PCBM in P3HT system. We interpret this as a step-in validation of the use of our approach for organic photovoltaic and support of its results for new systems that do not have reference data for comparison or calibration. For the less studied P3BT, our results show that expectations about its performance in binary blends with PCBM may be overestimated, as it does not demonstrate the required level of miscibility and short-range structural organization. The performance of P3BT with perovskites, however, seems as expected. The calculated nanoscale morphologies of blends of P3HT, P3BT or SQ with perovskites, including adsorption on TiO_2, are all new and serve as an instrument in rational design of organic/hybrid photovoltaics. They are used in collaboration with experts who make prototypes or devices for practical applications.

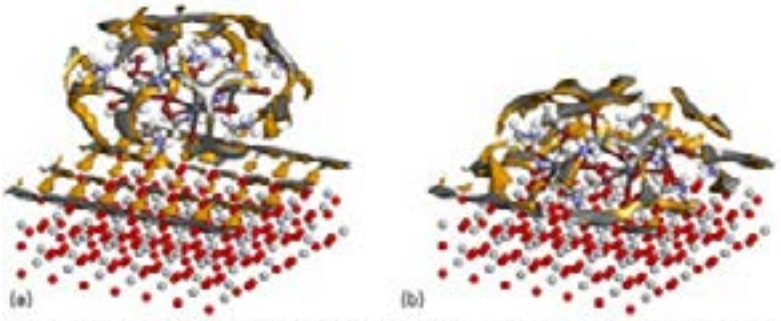

Figure 1. Modeling the morphology of $CH_3NH_3PbBr_3$ on TiO_2 in P3HT at T=400K: (a) small cluster away of surface; (b) close to it. Yellow and gray color isosurfaces show most probable locations of sulfur and carbon sites of P3BT around the perovskite cluster.

Biography

Alexander Kobryn has his expertise in predictive and descriptive modeling of equilibrium and time-dependent non-equilibrium phenomena in soft condensed matter systems such as molecular and macromolecular liquids and solutions, electrolytes and polyelectrolytes, gels and polymer blends, with the use of methods from statistical physics, theoretical physics, and theoretical and computational chemistry to research quantum and classical systems on multiple time and length scales, in nanoconfined geometries, and in nanoporous media. Successful applications include, in particular, polymer design rules for self-assembly of functionalized ionomers, explanation of the gelation mechanism and prefiguring of the gelation ability of multifunctional oligomeric electrolyte gelators, modeling of the active layer nanomorphology and dynamics of polymer blends that are building blocks for inexpensive organic and organic-metallic-halide solar panels, controlled fluid flow in MEMS and NEMS with CFD coupled to molecular properties of fluid and channel materials, etc.

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