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Tuning interfacial interactions between conjugated polymers and inorganic nanocrystals for control over bulk thermoelectric properties

BORIS RUSS, NELSON COATES, SHANNON YEE, Department of Chemical Engineering, University of California, Berkeley, CA and Lawrence Berkeley National Laboratory, Berkeley, CA, JEFFREY URBAN, Lawrence Berkeley National Laboratory, Berkeley, CA, RACHEL A. SEGALMAN, Department of Chemical Engineering, University of California, Berkeley, CA and Lawrence Berkeley National Laboratory, Berkeley, CA — Electronic transport in conjugated polymers is highly dependent on doping level and chain conformation. Recent advances in next-generation thermoelectric devices rely on the fabrication of conjugated-polymer:inorganic-nanocrystal composites, but little is known about the how the thermoelectric properties are influenced by the doping level or morphology of the conjugated polymer at the organic-inorganic interface. A thorough understanding of the coupling between the molecular orbitals of conjugated polymers and the energy states of inorganic materials in such systems is, therefore, paramount for achieving improvements in these devices. In this study, we present our results on the coupling between Poly-(3-hexylthiophene) (P3HT), a well-studied conjugated polymer, with solution-processed lead selenide (PbSe) nanocrystals of controlled shape and morphology. Conjugated oligomeric ligands are used to tailor the organic/inorganic interface between P3HT/PbSe. Our results address the effects of polymer conformation on the nanocrystal surface, polymer doping levels, and organic-inorganic energy level alignment on the bulk thermoelectric properties of these hybrid materials.

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