

Abstract Submitted
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First Principal Optimization of Exciton Separation via Functional Modification of the Atomic Structure LEVI LENTZ, ALEXIE KOLPAK, MIT — Low hole mobility and high recombination rates limit the incident photon-to-current collection efficiency (IPCE) of organic photovoltaics. In this study, we use a combination of rational design and first-principles density functional theory computations to tailor the properties of new hybrid organic-inorganic photovoltaic materials in order to ameliorate these issues. Starting with hybrid organic-inorganic molecules shown to self-assemble into crystalline structures, we design a nanostructured material in which inorganic charge carrier channels are separated by domains of organic absorber on the order of several nanometers thick perpendicular to the light absorption direction. By functionalizing the organic component and substituting the cations in the inorganic layer, we engineer a dipole moment to drive electrons and holes into the inorganic charge carrier channels. Furthermore, we tune the density of states of these regions via a combination of cation substitution and interactions with functional groups in the organic region in order to optimize charge carrier mobility. The combination of rational design and first-principles optimization could significantly reduce exciton recombination and increase charge carrier mobility with respect to purely organic photovoltaics.

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