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Functionalization of hybrid organic-inorganic materials for highly efficient photovoltaic materials LEVI LENTZ, ALEXIE KOLPAK, MIT — Low mobility and high recombination rates limit the incident photon conversion efficiency (IPCE) of organic-based photovoltaics. In this work we employ first-principles density functional theory calculations to investigate hybrid organic-inorganic materials designed to directly ameliorate these issues. By constructing superlattices composed of 2D transition metal phosphate sheets separated by ordered regions of well-known organic dyes, we show that one can significantly decrease recombination and increase charge carrier mobilities relative to typical organic photovoltaic materials. We discuss how functionalization of the molecules in the organic region can be used to simultaneously enhance exciton separation and tune the organic-inorganic band alignment to encourage charge transfer into the inorganic regions, which can act as high-mobility charge carrier channels. Our results suggest that nanostructured hybrid materials could significantly improve IPCE over traditional organic photovoltaics.

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