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2D Transition Metal Phosphates for use in the design of highly ordered organic bulk heterojunction photovoltaics

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Non-crystallinity of traditional bulk-heterojunction (BHJ) organic photovoltaic materials is one of the large limiters of their incident photon conversion efficiency (IPCE) because low carrier lifetimes and low diffusion lengths lead to a high rate of charge recombination. Transition metal phosphates (TMPs) are highly symmetric 2D materials that have been shown to be solution-processable with organic molecules due to out-of-plane trigonal phosphate groups. These structures have been studied for cation storage, however this ability to interact with organic structures creates a unique opportunity for BHJ applications. Using first principles simulations, we present a highly ordered BHJ structure using TMPs as control layers of existing organic semiconductors, overcoming the issues inherent to traditional BHJ materials. These intercalated TMP layers have much larger mobilites than organic semiconductors, allowing for effective charge extraction from the organic region, limiting the chances of recombination of excitons. Further, the designed system allows for precise control of the organic molecule size, minimizing the size of the organic region to a length much smaller than typical exciton diffusion lengths observed in BHJs. Using organic functional groups, the organic semiconductor can be functionalized to control polarity, allowing dipole engineering to overcome the exciton binding energy in the molecule, eliminating the need for energetic differences to separate the bound charge, maximizing the VOC of the material. This dipole also allows for control of the energetic levels of the TMPs layers, driving electrons and holes into different layers, minimizing the presence of minority carriers in the TMP layers, further decreasing the chance of recombination. This combination of molecular design elements allows for atomic engineering to maximize the total efficiency of highly studies organic semiconductors used in photovoltaic applications.

Keywords: photovoltaic; organic; phosphate; recombination; superstructure