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Modeling recombination processes and predicting energy conversion efficiency of dye sensitized solar cells from first principles WEI MA, SHENG MENG, Chinese Academy of Sci (CAS) — We present a set of algorithms based on solo first principles calculations, to accurately calculate key properties of a DSC device including sunlight harvest, electron injection, electron-hole recombination, and open circuit voltages. Two series of D-π-A dyes are adopted as sample dyes. The short circuit current can be predicted by calculating the dyes' photo absorption, and the electron injection and recombination lifetime using real-time time-dependent density functional theory (TDDFT) simulations. Open circuit voltage can be reproduced by calculating energy difference between the quasi-Fermi level of electrons in the semiconductor and the electrolyte redox potential, considering the influence of electron recombination. Based on timescales obtained from real time TDDFT dynamics for excited states, the estimated power conversion efficiency of DSC fits nicely with the experiment, with deviation below 1-2%. Light harvesting efficiency, incident photon-to-electron conversion efficiency and the current-voltage characteristics can also be well reproduced. The predicted efficiency can serve as either an ideal limit for optimizing photovoltaic performance of a given dye, or a virtual device that closely mimicking the performance of a real device under different experimental settings.

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