THE CHINESE UNIVERSITY OF HONG KONG

Department of Physics

SEMINAR

Multi-Scale Theoretical Simulations of Organic Photovoltaic and Organic-Inorganic Hybrid Perovskite Materials

by

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ALL INTERESTED ARE WELCOME
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Abstract

Over the past several years, the power conversion efficiencies (PCE) of single-junction organic solar cells (OSCs) have jumped from 11% to 19%. However, the PCE values of the most efficient OSCs remain significantly smaller than those values of inorganic and hybrid perovskite solar cells. One of the major reasons is the much larger voltage losses due to non-radiative charge recombination. Here, we thus employed multi-scale theoretical approaches integrating density functional theories (DFT), vibronic theories, and all-atom molecular dynamics (AA-MD) to (i) establish relationship between excitonic properties of OSC active materials and non-radiative voltage loss, and (ii) understand impact of molecular structures and intermolecular packing/orientations on non-radiative voltage loss. In addition to organic solar cells, we also utilized DFT combined with non-adiabatic molecular dynamics to evaluate the different impacts that the 2D-confined spacer layer of butylammonium cations and the 3D-confined methylammonium cations have on the charge carrier dynamics in the two systems.

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