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理论研究 BBPQ-PC_{61}BM 体系的光伏性质

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Theoretical Investigation on Photovoltaic Properties of the BBPQ-PC_{61}BM System

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Fig. S1  Relative energy of BBPQ-PC$_{61}$BM complex as a function of the centroids distance of BBPQ and PC$_{61}$BM

Fig. S2  Relative energy of BBPQ-PC$_{61}$BM complex as a function of the orientation angle ($\theta$) of BBPQ and PC$_{61}$BM
Fig. S3  Optimized BBPQ structure at the CAM-B3LYP/6-311G(d,p) level

Fig. S4  Energy evolution as a function of the centroids distance of face-to-face BBPQ dimer
Fig.S5  Energy evolution as a function of the orientation angle ($\theta$) of face-to-face BBPQ dimer

The detailed description for molecular dynamics simulation

As seen in Eq(8), to estimate the $\lambda_{\text{ext}}$, the optical dielectric constant of medium, $\varepsilon_{\text{opt}}$, needs to be calculated by means of Eq(9), that is to say, we firstly need to estimate the material’s density $\rho$. Here, Materials Studio 5.5 software package was applied. The simulation process included four basic steps, which were described as following according to previous studies\textsuperscript{1-3}.

Firstly, the BBPQ molecule was optimized at the CAM-B3LYP/6-311G(d,p) level with Gaussian 09 software (Fig. S6), and then the stable molecule was introduced the Materials studio 5.5 software package. Then, the Compass force field and Amorphous Cell module were applied to establish an amorphous cell containing 50 BBPQ molecules. And then, the Discover module and smart minimizer method were used to roughly optimize the amorphous cell more than 5000 steps.

Thus, a relatively reasonable amorphous cell (I) was obtained (Fig. S7).

Fig.S6  Optimized BBPQ at the CAM-B3LYP/6-311G(d,p) level

S4
Secondly, the cell (I) was introduced into the Forcite Module, and increased its temperature from 200 K to 600 K, and then decreased it from 600 K to 200 K. After the two-step annealing processing including 10 cycles, the unreasonable structures were efficiently eliminated. Then, the stable cell (II) was obtained, which provided a relatively balance geometry for the subsequent molecular dynamics simulation. Fig.S8 showed the energy variation of amorphous cell with the simulated time. Fig.S9 exhibited the temperature change with the simulated time.
Thirdly, in order to achieve the equilibrium state as soon as possible, a molecular dynamics simulation with 200ps under the condition of constant volume and constant temperature (NVT) was firstly carried out. In the practical simulation, the Compass force field and the current charge were applied. Finally, the amorphous cell (III) was obtained. Fig.S10 showed the energy variation of amorphous cell with the simulated time. Fig.S11 exhibited the temperature change with the simulated time. As seen, when the simulated time was over 10ps, the cell was close to be stable.

Fourthly, based on the cell structure obtained by means of the step 3, a molecular dynamics simulation for 500ps under the condition of constant pressure and temperature constant (NPT) was carried out, after 200ps the system was balanced, finally, the material density was obtained (Fig.S13). In the practical simulation, the Compass force field and the current charge were applied. In addition, the total simulated time was selected to 500ps. Fig.S12 showed the structural variation of amorphous cell with the simulated time. Fig.S13 exhibited the material’s density change with the simulated time. As seen, when the simulated time is over 200ps, the cell trends toward to be stable.
Fig. S12  Correlation of structures and time in NPT simulation

Fig. S13  Correlation of density and time in NPT simulation

