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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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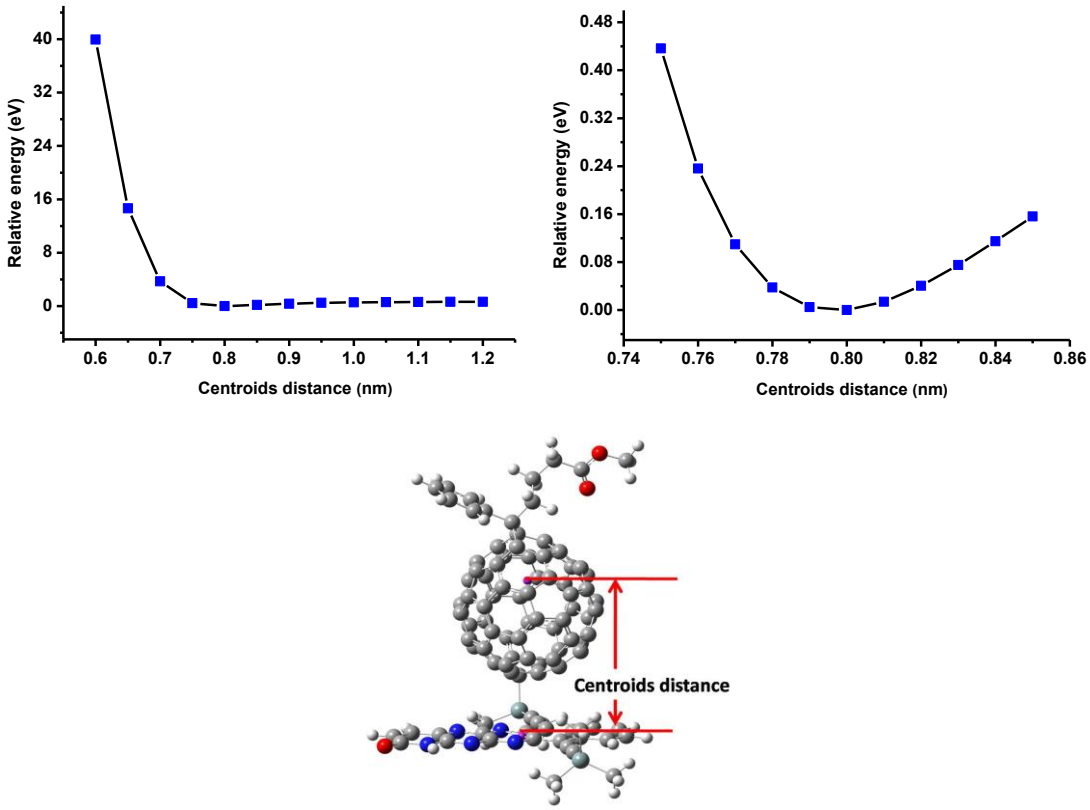

Fig.S1 Relative energy of BBPQ-$PC_{61}BM$ complex as a function of the centroids distance of BBPQ and $PC_{61}BM$

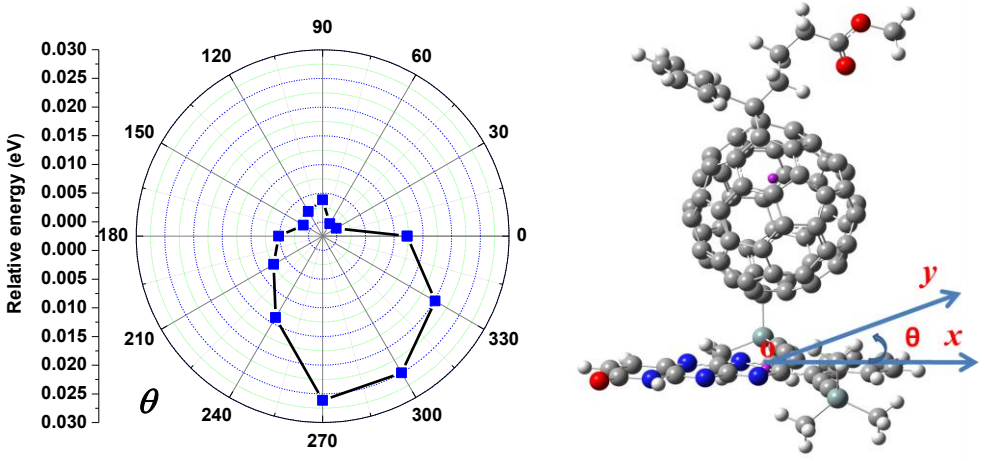

Fig.S2 Relative energy of BBPQ-$PC_{61}BM$ complex as a function of the orientation angle (θ) of BBPQ and $PC_{61}BM$

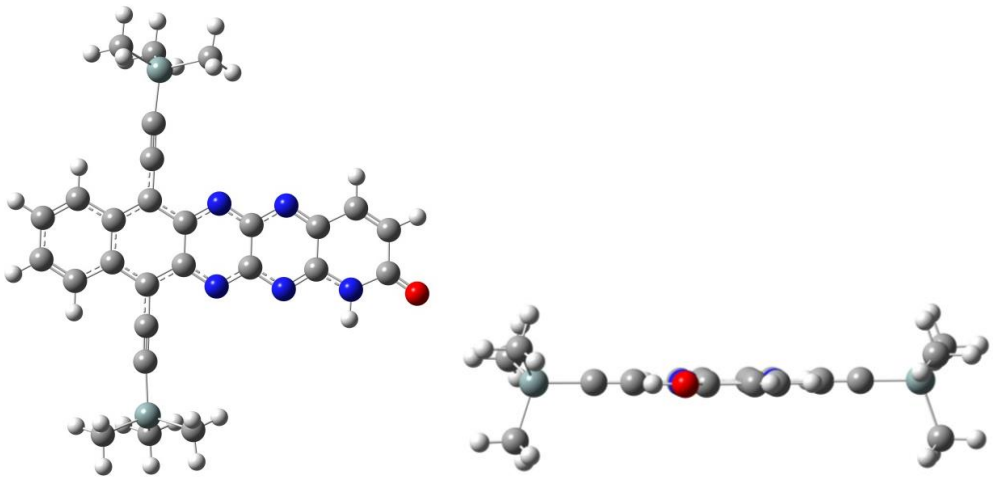

Fig.S3 Optimized BBPQ structure at the CAM-B3LYP/6-311G(*d*,*p*) level

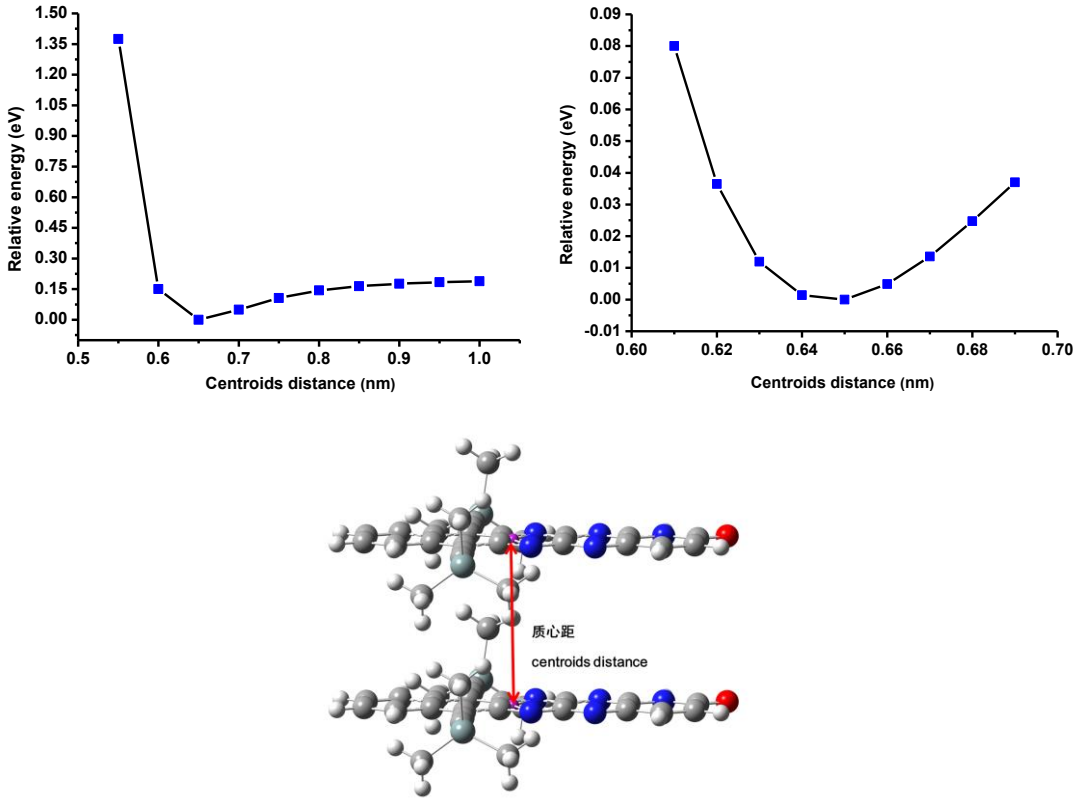

Fig.S4 Energy evolution as a function of the centroids distance of face-to-face BBPQ dimer

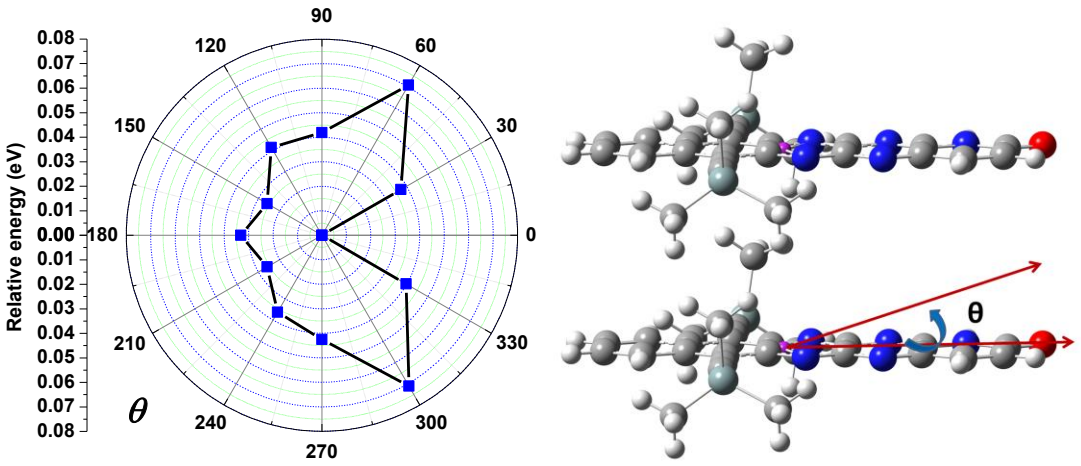

Fig.S5 Energy evolution as a function of the orientation angle (*θ*) of face-to-face BBPQ dimer

The detailed description for molecular dynamics simulation

As seen in Eq(8), to estimate the λ_{ext}, the optical dielectric constant of medium, ε_{op}, needs to be calculated by means of Eq(9), that is to say, we firstly need to estimate the material's density ρ. 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[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).

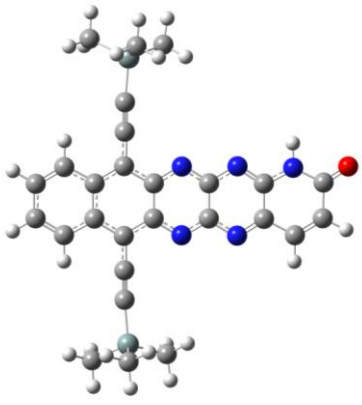

Fig.S6 Optimized BBPQ at the CAM-B3LYP/6-311G(*d*,*p*) level

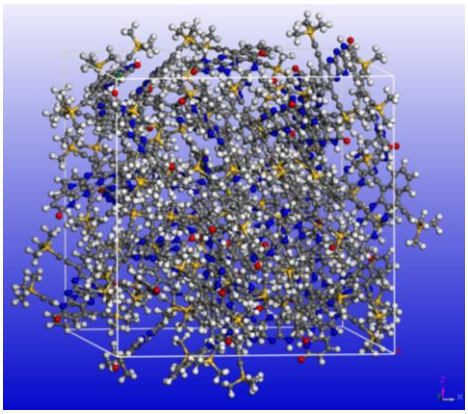

Fig.S7 Optimized amorphous cell including 50 BBPQ molecules

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 600K 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.

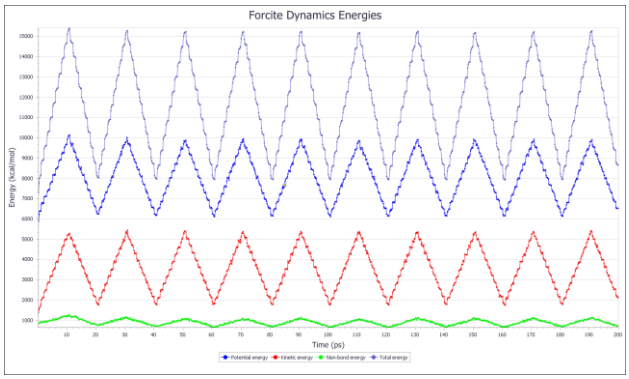

Fig.S8 Correlation of energy and time in annealing simulation

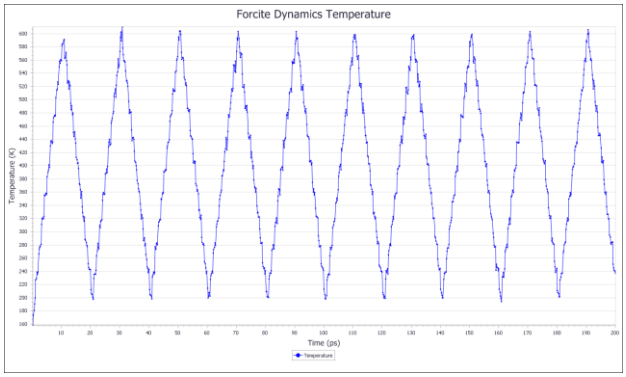

Fig.S9 Correlation of temperature and time in annealing simulation

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.

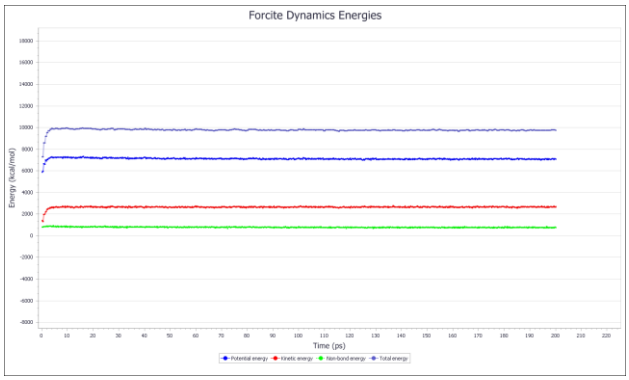

Fig.S10 Correlation of energy and time in NVT simulation

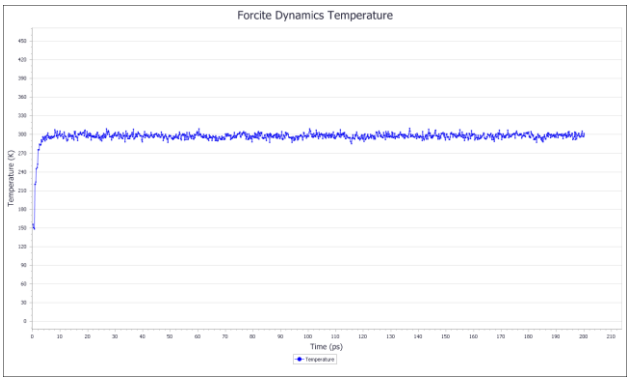

Fig.S11 Correlation of temperature and time in NVT simulation

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.

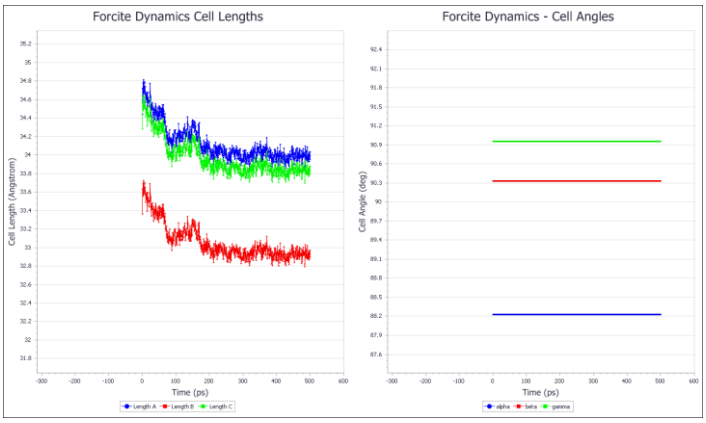

Fig.S12　Correlation of structures and time in NPT simulation

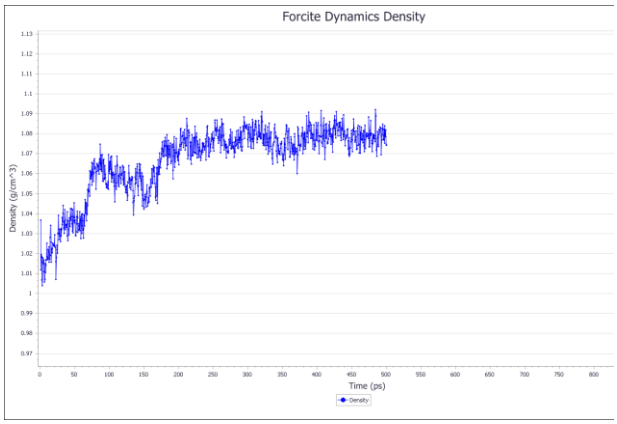

Fig.S13　Correlation of density and time in NPT simulation

(1) Fu, Y. Z.; Liu, Y. Q.; Lan, Y. H. *Acta Phys. -Chim. Sin.* **2009,** *25*, 1267. [付一政，刘亚青，兰艳花．物理化学学报, **2009**, *25*, 1267.] doi: 10.3866/PKU.WHXB20090710

(2) Sun, D. L.; Zhou, J. *Acta Phys. -Chim. Sin.* **2012,** *28*, 909. [孙德林，周健．物理化学学报, **2012,** *28*, 909.] doi: 10.3866/PKU. WHXB201201164

(3) Zhao, G. Z.; Feng, Y. B.; Fu, Fu, Y. Z.; Lan, Y. H.; Liu, Y. Q. *Acta Chim. Sin.* **2009,** *67*, 2233. [赵贵哲，冯益柏，付一政，兰艳花，刘亚青．化学学报, **2009,** *67*, 2233.]