Supporting Information

Revealing the interactions between pentagon-octagon-pentagon defect graphene and organic donor/acceptor molecules: a theoretical study

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SI 1: The visualization details:

The wave-functions were generated by Gaussian09 [1] at wb97xd/tzvp level based on one unit cell ended with hydrogen.

Multiwfn2.6 deals with reduced density gradient (RDG) in real space as equal 1:

$$RDG(r) = \frac{1}{2*(3*\pi^2)^{\frac{1}{3}}} * \frac{|\nabla\rho(r)|}{\rho(r)^{\frac{4}{3}}} \quad (1)$$

Where ρ(r) is electron density and can be defined as equal 2， $\nabla\rho(r)$ is the electron density gradient.

$$\rho(r) = \sum_i \eta_i |\varphi_i(r)|^2 = \sum_i \eta_i \left| \sum_l C_{l,i} \chi_l(r) \right|^2 \quad (2)$$

Where φ is orbital wave function generated by wb97xd/tzvp mentioned above, η_i is occupation number of orbital *i*, χ is basis function. *C* is coefficient matrix, the element of i^{th} row j^{th} column corresponds to the expansion coefficient of orbital *j* respect to basis function *i*. The other details of Multiwfn2.6 are in the web: http://multiwfn.codeplex.com/

Table SI2. The lattice parameters of pristine and defected graphene models. a) Accurately, there have very slight difference form 90.000°.

Lattice	Pristine graphene (Å)	Defect graphene (Å)
a axis	14.760	14.253
b axis	12.780	12.977
α angle	90.000	90.001
β angle	90.000	90.000[a]
γ angle	90.000	90.000[a]

Configurations	Energy (ev)	Configurations	Energy (ev)

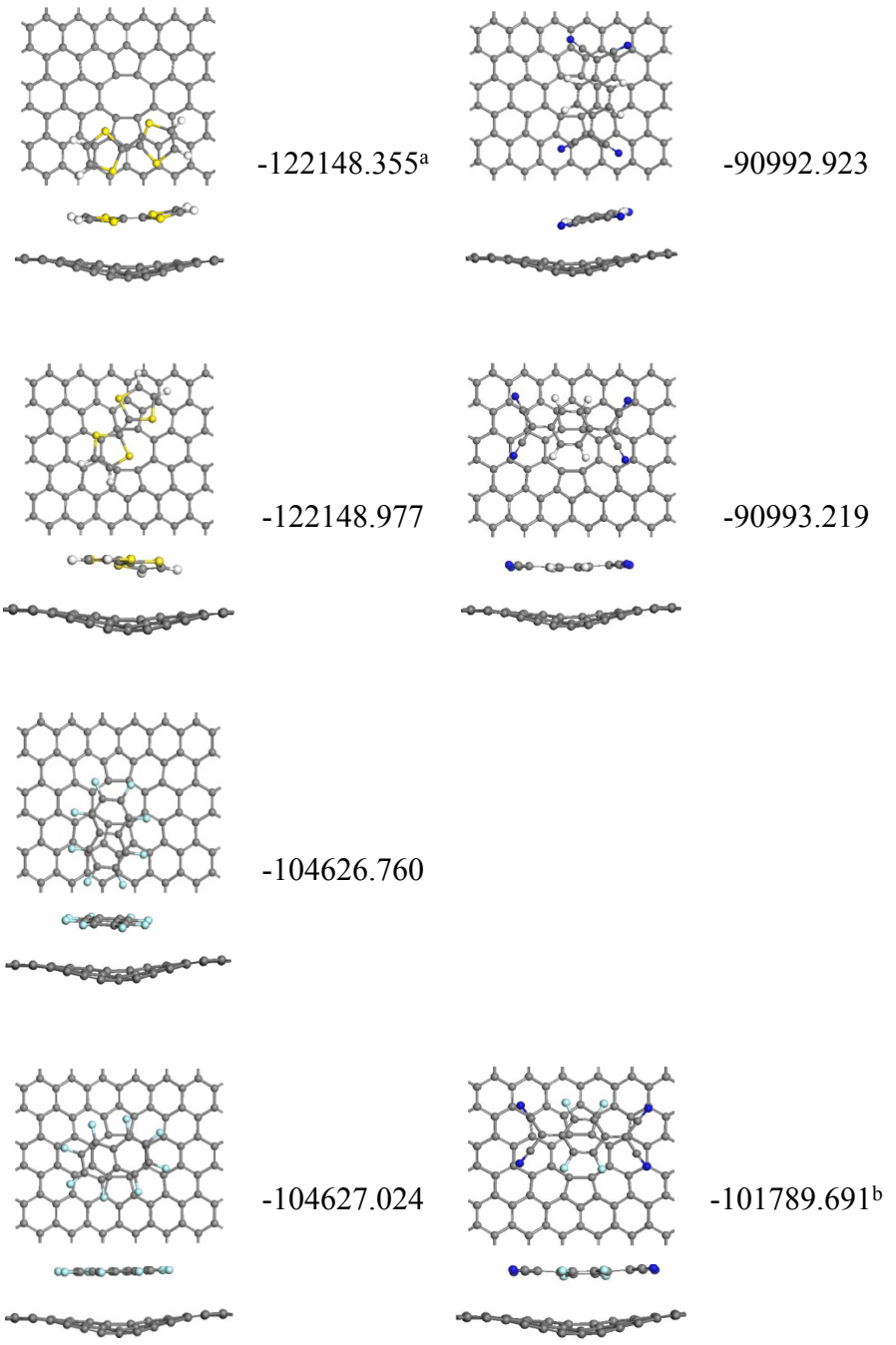

Figure SI3. The relatively stable configurations and total energies of DG-TTF and DG-FNa (left), DG-TCNQ and DG-F4TCNQ (right). [a]This configuration of DG-TTF cannot be converged at SCF tolerance 1.0e-6 Ha, max force 2.0e-3 Ha/Å and max displacement 0.005 Å level, it was obtained at SCF tolerance 1.0e-5 Ha; [b]DG-F4TCNQ was constructed basing on DG-TCNQ.

Table SI4. The interaction energy (eV) between DG and D/A molecules calculated by

GGA/PBE-TS[a] and GGA/PBE-Grimme[b] method with DNP basis and 6×6×6 k-points in Dmol[3] module. The interaction energy calculated by TS correction is about 0.3 eV bigger than Grimme.

	Interaction energy (eV)[a]	Interaction energy (eV)[b]
DG-TTF	-1.28	-0.92
DG-FNa	-1.15	-0.89
DG-TCNQ	-1.55	-1.20
DG-F4TCNQ	-1.81	-1.49

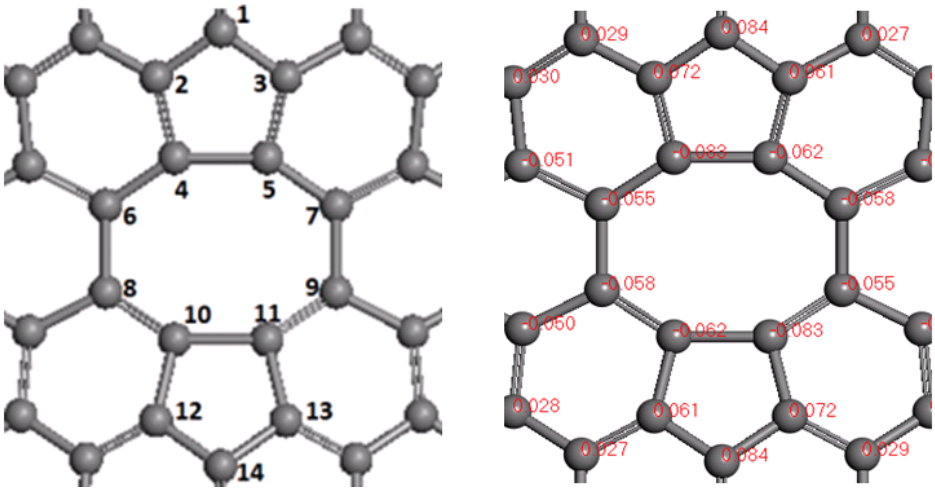

Figure SI5. The 14 atoms in defect part (left), charge distribution (right) calculated in Dmol[3] module by GGA/PBE-TS method. The charges of atom 1-14 are: 0.084, 0.072, 0.061, -0.083, -0.062, -0.055, -0.058, -0.058, -0.055, -0.062, -0.083, 0.061, 0.072, 0.084 e respectively.

References

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