Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics
This journal is © The Owner Societies 2011

Supporting information

Density Functional Study on the Increment of Carrier Mobility in Armchair Graphene Nanoribbons Induced by Stone-Wales Defects

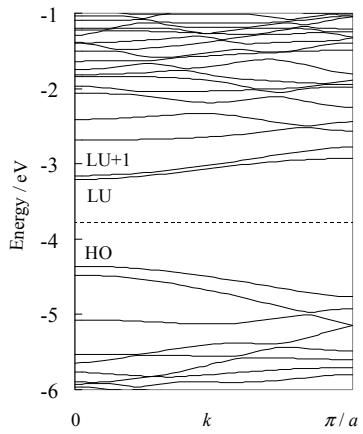
Guo Wang

Department of Chemistry, Capital Normal University, Beijing 100048, China.

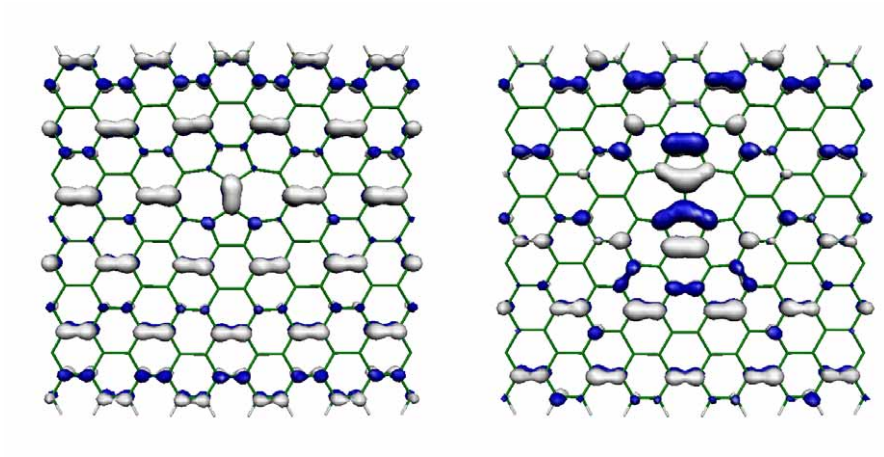
E-mail: wangguo@mail.cnu.edu.cn

Table S1 Stretching modulus C(eVÅ^{-1}), hole effective mass m_h^*, electron effective mass m_e^*(m_0), valence band deformation potential constant E_{1v}, conduction band deformation potential constant E_{1c}(eV), hole mobility μ_h, and electron mobility μ_e(cm^{2}V^{-1}s^{-1}) of the graphene nanoribbons calculated with different methods.

Nomenclature	Method	C	$\|m_h^*\|$	$\|m_e^*\|$	E_{1v}	E_{1c}	μ_h	μ_e
armchair9	B3LYP/6-21G(d, p)	294	0.09	0.08	12.0	3.1	656	9767
	B3LYP/3-21G(d, p)	232	0.08	0.08	12.1	3.2	512	7630
	PBE/6-21G(d, p)	292	0.09	0.09	10.1	1.6	844	32320
	PBE/SZP(SIESTA)	217	0.09	0.09	7.6	3.7	1042	4386
armchair17	B3LYP/6-21G(d, p)	548	0.06	0.06	5.2	13.0	12259	1941
	B3LYP/3-21G(d, p)	499	0.06	0.06	5.3	10.9	10679	2516
	PBE/6-21G(d, p)	460	0.08	0.08	2.6	10.2	24393	1513
	PBE/SZP(SIESTA)	410	0.08	0.08	4.5	7.1	7863	3069
armchair9-5cellSW	B3LYP/6-21G(d, p)	268	0.06	0.05	10.9	2.7	1384	24575
	PBE/6-21G(d, p)	264	0.05	0.05	8.9	1.1	2211	105020



(a)



(b) (c)

Fig. S1 (a) Band structures of armchair16-5cellSW, (b) HOCO, and (c) LUCO of armchair16-5cellSW.

For most structures with Stone-Wales defects, the deformation potential has only a little change compared with the perfect nanoribbons. However, for armchair13-5cellSW and armchair16-5cellSW, E_{1c} is only a quarter of the value for the corresponding perfect nanoribbon. From Fig. S1(a), it can be seen that the LU and LU+1 bands of armchair16-5cellSW are quite close to each other. The interaction between the two bands changes the LUCO shown in Fig. S1(c), which is not localized with respect to the one-dimensional deformation direction. The deformation potential constant E_{1c} decreases much. The HOCO shown in Fig. S1(b) is still delocalized compared with that of armchair16, so E_{1v} changes little. For armchair13-5cellSW, the situation is similar.