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Supplementary Information

Electron Transport Study on Functionalized Armchair Graphene Nanoribbons: DFT Calculations

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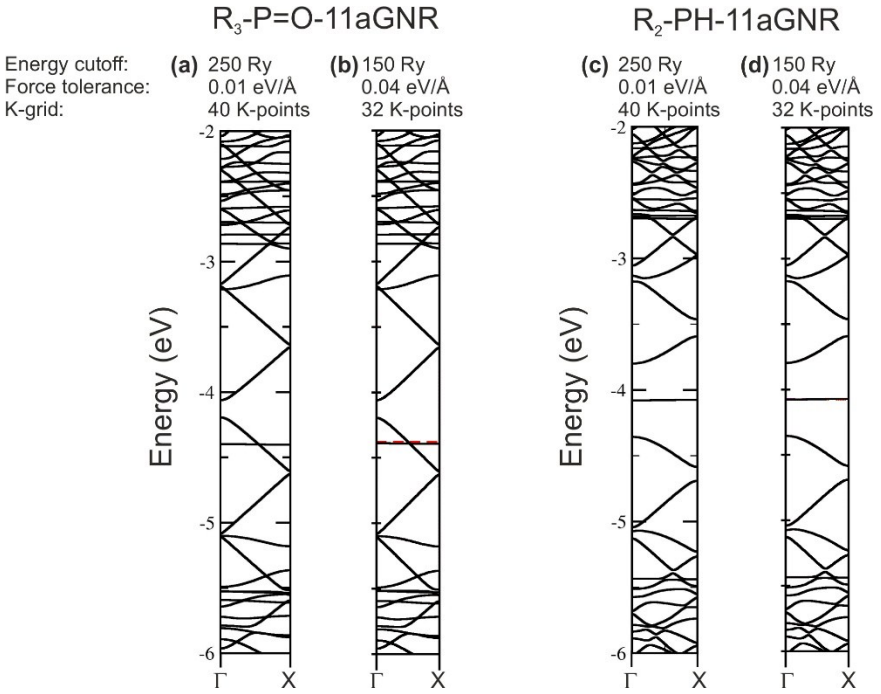

Figure S1: Band structure of **(a-b)** inside R_3-P=O-11aGNR and **(c-d)** edge R_2-PH-11aGNR with different computation parameters.

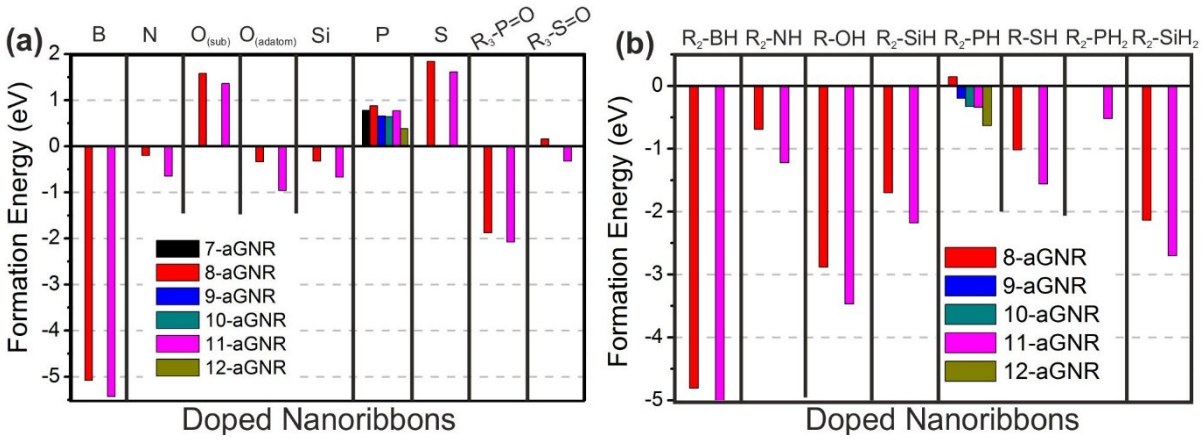

Figure S2: Formation energy of 42 armchair nanoribbons doped at the **(a)** inside and **(b)** edge. Note negative values indicate energetically favourable structures.

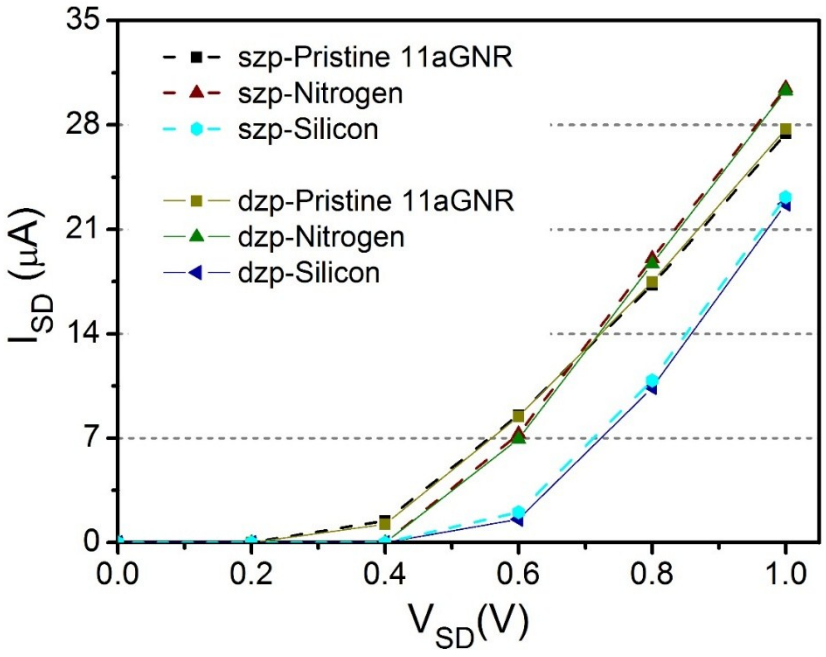

Figure S3: Current-Voltage (I-V) characteristics of undoped-, N- and Si-doped 11-aGNRs comparing the effect of using single ζ-plus-polarization basis (SZP) and double ζ-plus-polarization basis (DZP).

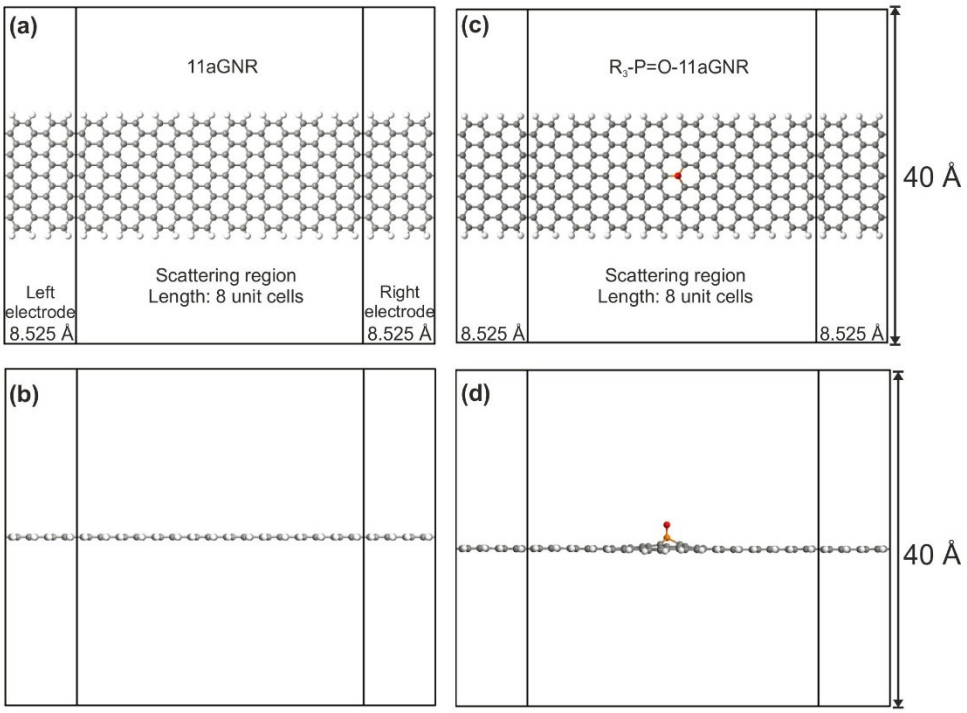

Figure S4: Devices used to determine the I-V characteristics. **(a-b)** Top and side view of the pristine 11-aGNR. **(c-d)** Top and side view of the R_3-P=O-11aGNR. Other systems has a similar configuration.

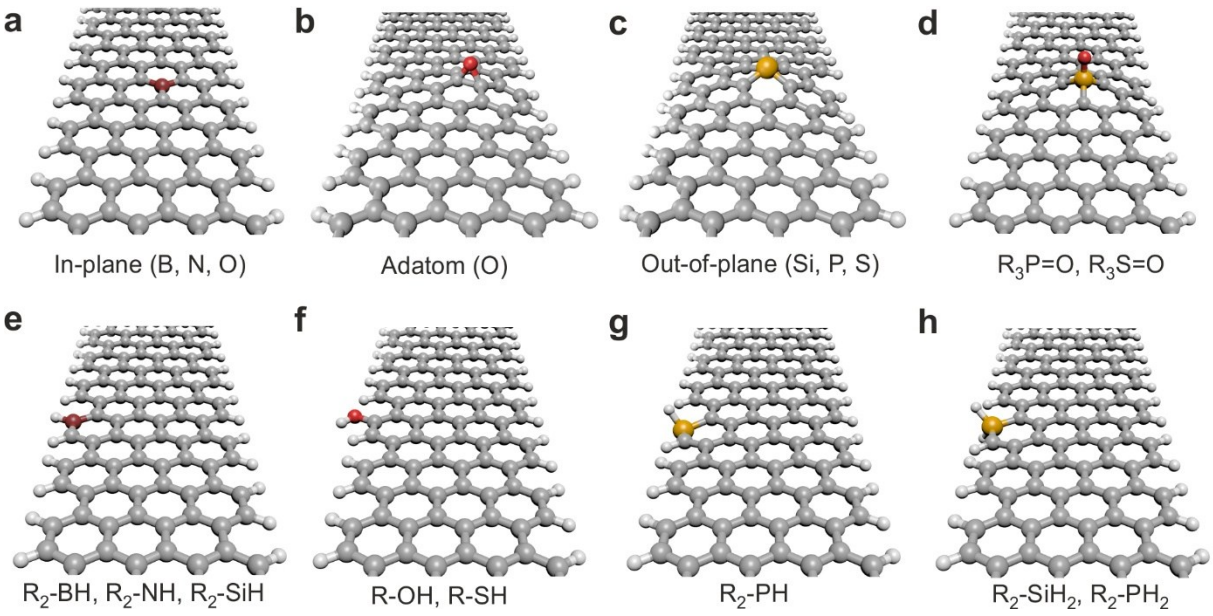

Figure S5: (a-d) Inside-doped and **(e-h)** edge-doped 8-aGNRs.

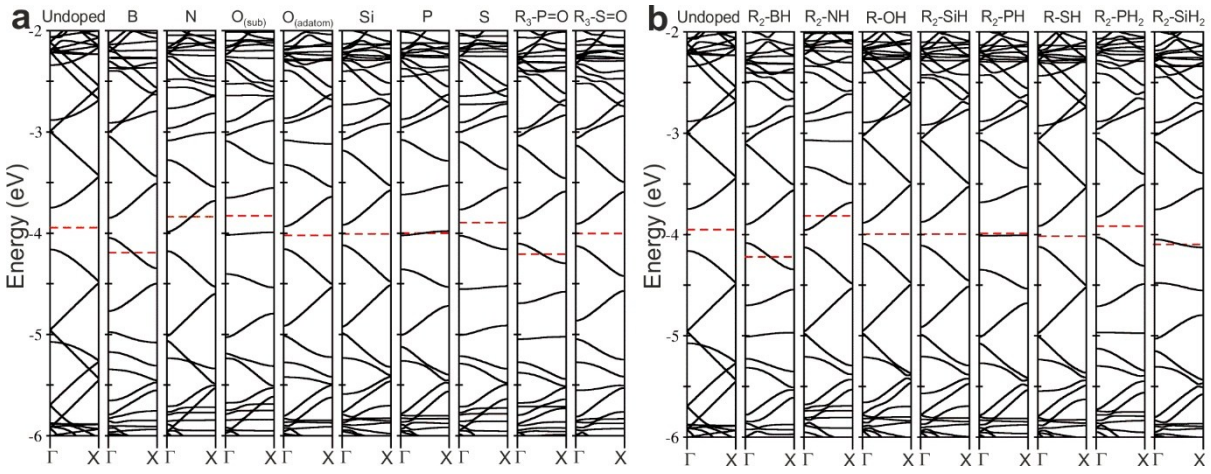

Figure S6: Band structure plots of 8-aGNRs. **(a)** Inside-doped, and **(b)** edge-doped systems. The Fermi level is indicated with a red dashed line.

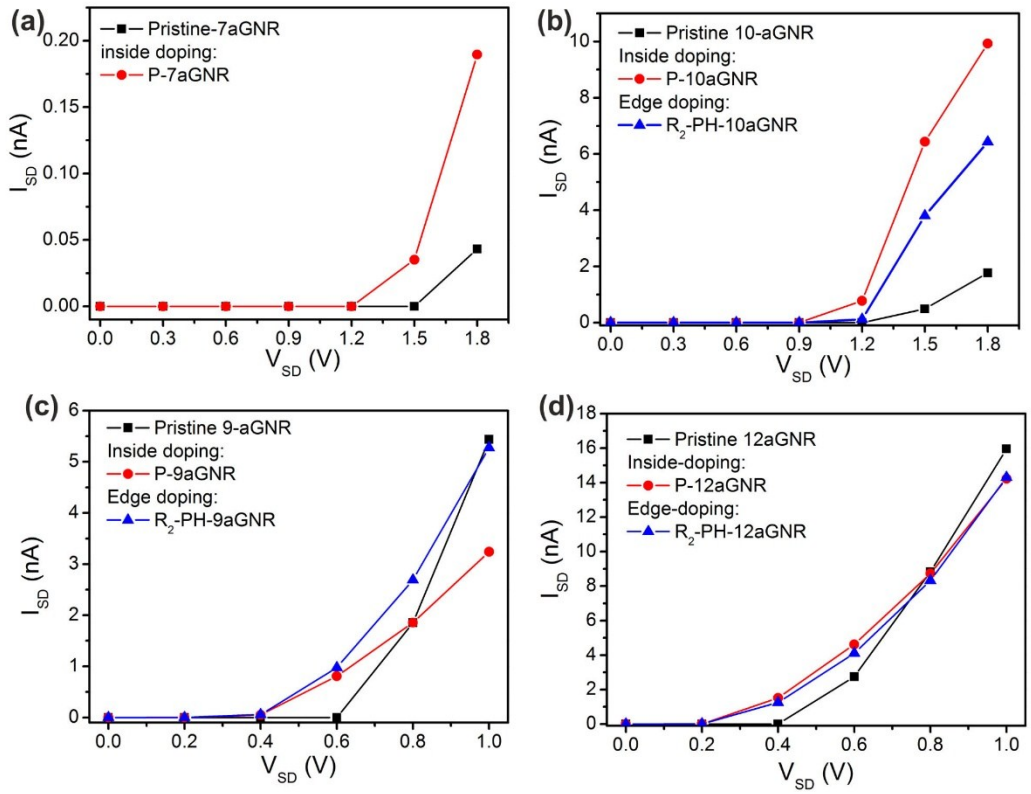

Figure S7: I-V curves of **(a)** 7- and **(b)** 10-aGNRs (3p family). **(c)** 9- and **(d)**-12aGNR (3p+1 family) with a phosphorous-inside (P-) doping and the corresponding edge case (R_2-PH-).

Table S1: Lattice expansion and electronic band gap (E_g) of doped and undoped 11-aGNRs.

Inside-doped 11-aGNR			**Edge-doped 11-aGNR**		
Dopant	**Lattice expansion (%)**	**E_g (eV)**	**Dopant**	**Lattice expansion (%)**	**E_g (eV)**
Pristine	-**	0.331	Pristine	-**	0.331
Boron	1.68	*p*-doped	R_2-BH	1.60	*p*-doped
Nitrogen	1.54	*n*-doped	R_2-NH	1.56	*n*-doped
Oxygen (Sub)	1.54	*	R-OH	1.50	0.150
Oxygen (Adatom)	1.54	0.159			
Silicon	1.74	0.158	R_2-SiH	1.70	0.169
Phosphorous	1.66	*	R_2-PH	1.68	*
Sulfur	1.66	0.150	R-SH	1.55	0.150
R_3-P=O	1.66	*	R_2-PH_2	1.68	0.152
R_3-S=O	1.66	0.161	R_2-SiH_2	1.70	*

*Flat bands at the Fermi level
** Initial lattice parameter 34.10064 Å

Table S2: Lattice expansion and electronic band gap (E_g) of doped and undoped 8-aGNRs.

Center-doped 8-aGNR			**Edge-doped 8-aGNR**		
Dopant	**Lattice expansion (%)**	**E_g (eV)**	**Dopant**	**Lattice expansion (%)**	**E_g (eV)**
Pristine	-**	0.413	Pristine	-**	0.413
Boron	1.92	*p*-doped	R_2-BH	1.86	*p*-doped
Nitrogen	1.73	*n*-doped	R_2-NH	1.74	*n*-doped
Oxygen (sub)	1.77	0.368	R-OH	1.80	0.206
Oxygen (Adatom)	1.78	0.221			
Silicon	2.02	0.202	R_2-SiH	1.95	0.222
Phosphorous	1.93	*	R_2-PH	1.92	*
Sulfur	1.86	0.219	R-SH	1.78	0.202
R_3-P=O	1.95	-	R_2-PH_2	1.95	0.204
R_3-S=O	1.86	0.218	R_2-SiH_2	1.92	*

*Flat bands at the Fermi level
**Initial lattice parameter 34.10064 Å

Table S3: Magnetic moment on system with half-filled bands.

Doped 11-aGNR	**Magnetic moment (μ_B)**
$O_{(Sub)}$	0.3
P	1.0
R_3-P=O	0.1
Si	0.0
R_2-PH	1.0