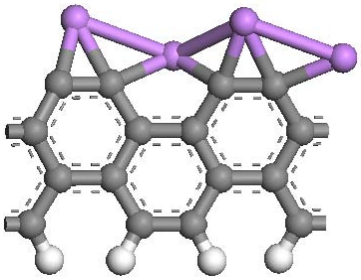
Supporting Information

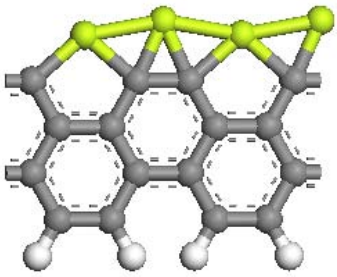
Table S1. Covalent radii and M-M bond length of various elements**.**

Elements	**Li**	**Be**	**B**	**N**	**O**	**F**
Covalent radii (Å)	1.28	0.96	0.84	0.71	0.66	0.57
M-M bond length (Å)	3.04	2.22	1.59	1.10	1.21	1.42
Elements	**Na**	**Mg**	**Al**	**Si**	**P**	**S**
Covalent radii (Å)	1.66	1.41	1.21	1.11	1.07	1.05
M-M bond length (Å)	3.72	3.20	2.86	2.35	2.21	2.05
Elements	**Cl**	**K**	**Ca**	**Sc**	**Ti**	**V**
Covalent radii (Å)	1.02	2.03	1.74	1.70	1.60	1.53
M-M bond length (Å)	1.89	4.54	3.95	3.21	2.90	2.62
Elements	**Cr**	**Mn**	**Fe**	**Co**	**Ni**	**Cu**
Covalent radii (Å)	1.39	1.39	1.32	1.26	1.24	1.32
M-M bond length (Å)	2.50	2.73	2.48	2.51	2.49	2.56
Elements	**Zn**	**Ga**	**Ge**	**As**	**Se**	**Br**
Covalent radii (Å)	1.22	1.22	1.20	1.19	1.20	1.20
M-M bond length (Å)	2.67	2.44	2.45	2.49	2.32	2.28
Elements	**Ag**	**Au**				
Covalent radii (Å)	1.45	1.36				
M-M bond length (Å)	2.89	2.88				

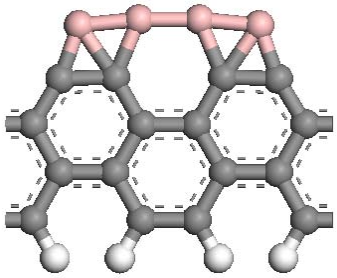
Figure S1. Stable configurations of atoms-decorated armchair graphene nanoribbon (AGNR).



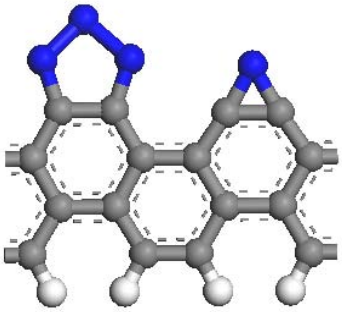
(1) Li $_{(C1)}$



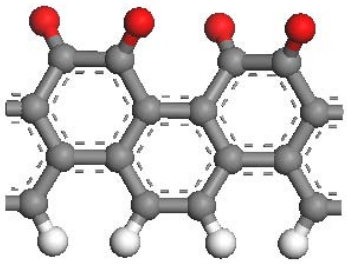
(2) Be $_{(Cs)}$



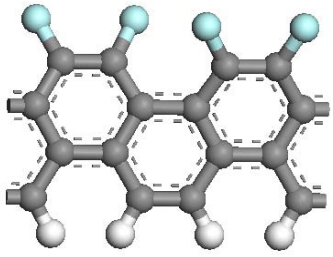
(3) B $_{(Cs)}$



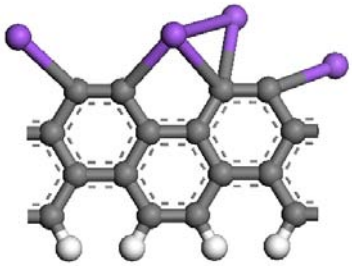
(4) N $_{(Cs)}$



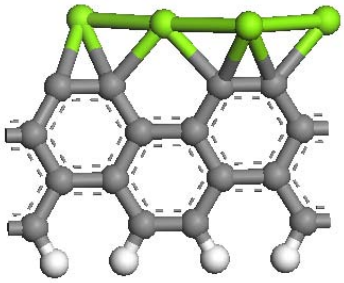
(5) O $_{(C1)}$



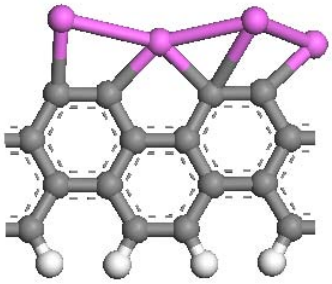
(6) F $_{(C1)}$



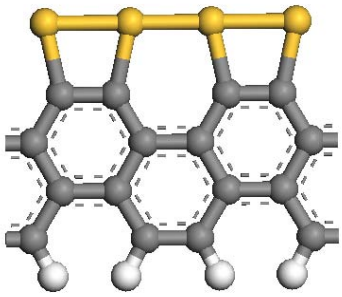
(7) Na $_{(C1)}$



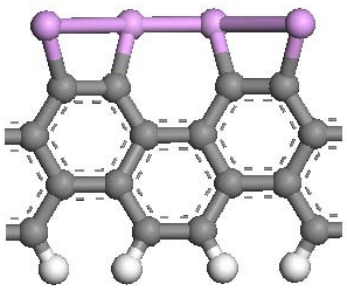
(8) Mg $_{(C1)}$



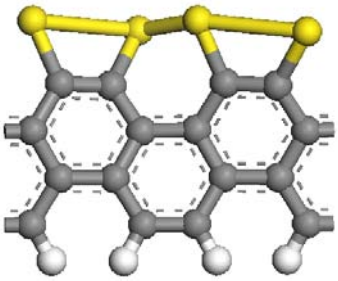
(9) Al $_{(C1)}$



(10) Si $_{(Cs)}$

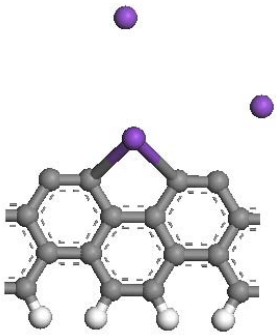


(11) P $_{(C1)}$

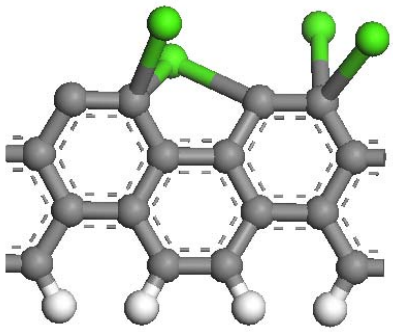


(12) S $_{(C1)}$

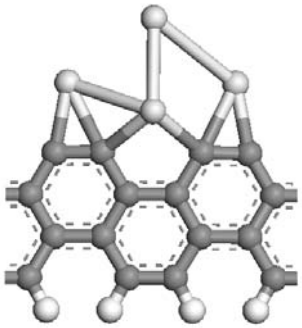
Figure S1 (continued)



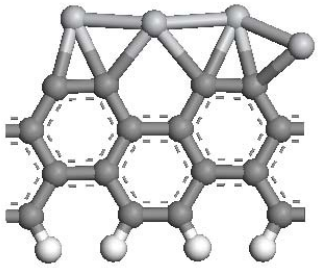
(13) K (C1)



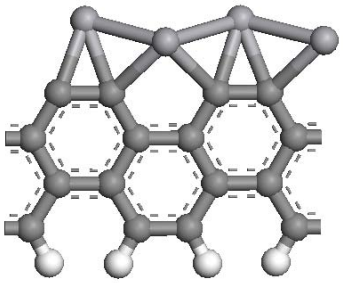
(14) Ca (C1)



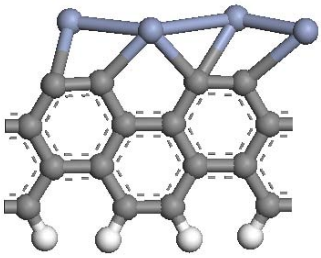
(15) Sc (C1)



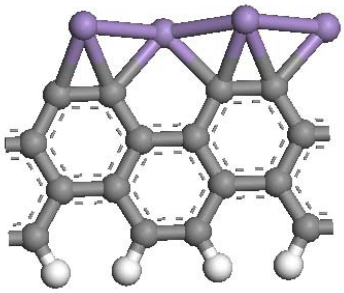
(16) Ti (C1)



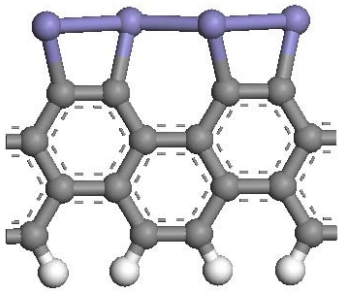
(17) V (C1)



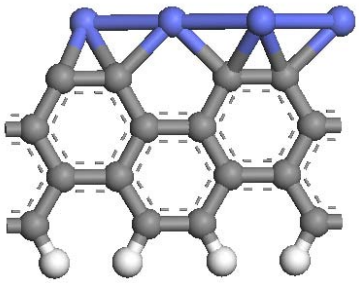
(18) Cr (C1)



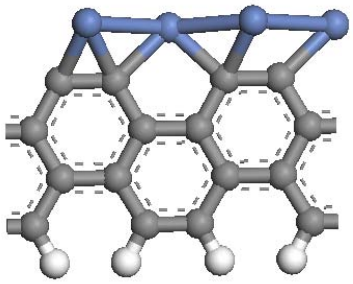
(19) Mn (Cs)



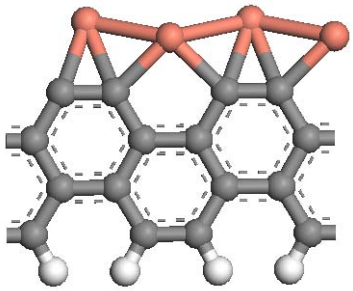
(20) Fe (C1)



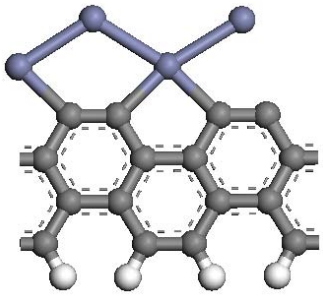
(21) Co (C1)



(22) Ni (C1)

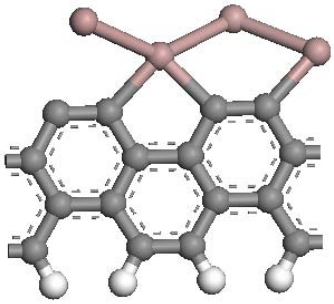


(23) Cu (C1)

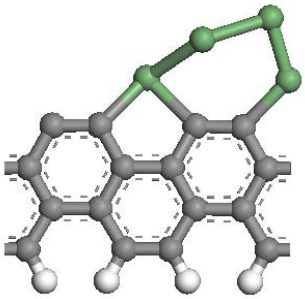


(24) Zn (Cs)

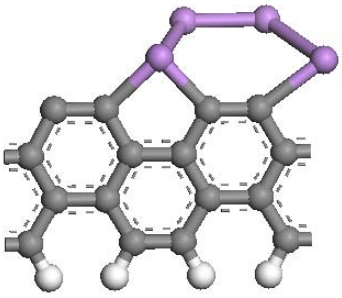
Figure S1 (continued)



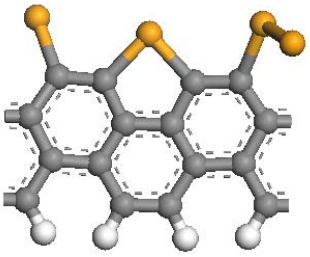
(25) Ga $_{(C1)}$



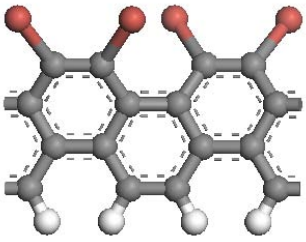
(26) Ge $_{(C1)}$



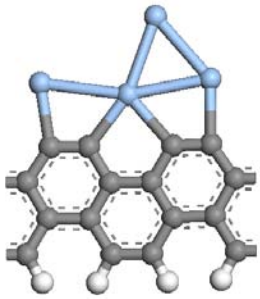
(27) As $_{(C1)}$



(28) Se $_{(C1)}$



(29) Br $_{(C1)}$



(30) Ag $_{(Cs)}$

(31) Au $_{(Cs)}$

Figure S2. Various initial configurations for the adsorption of Be atoms on AGNR.

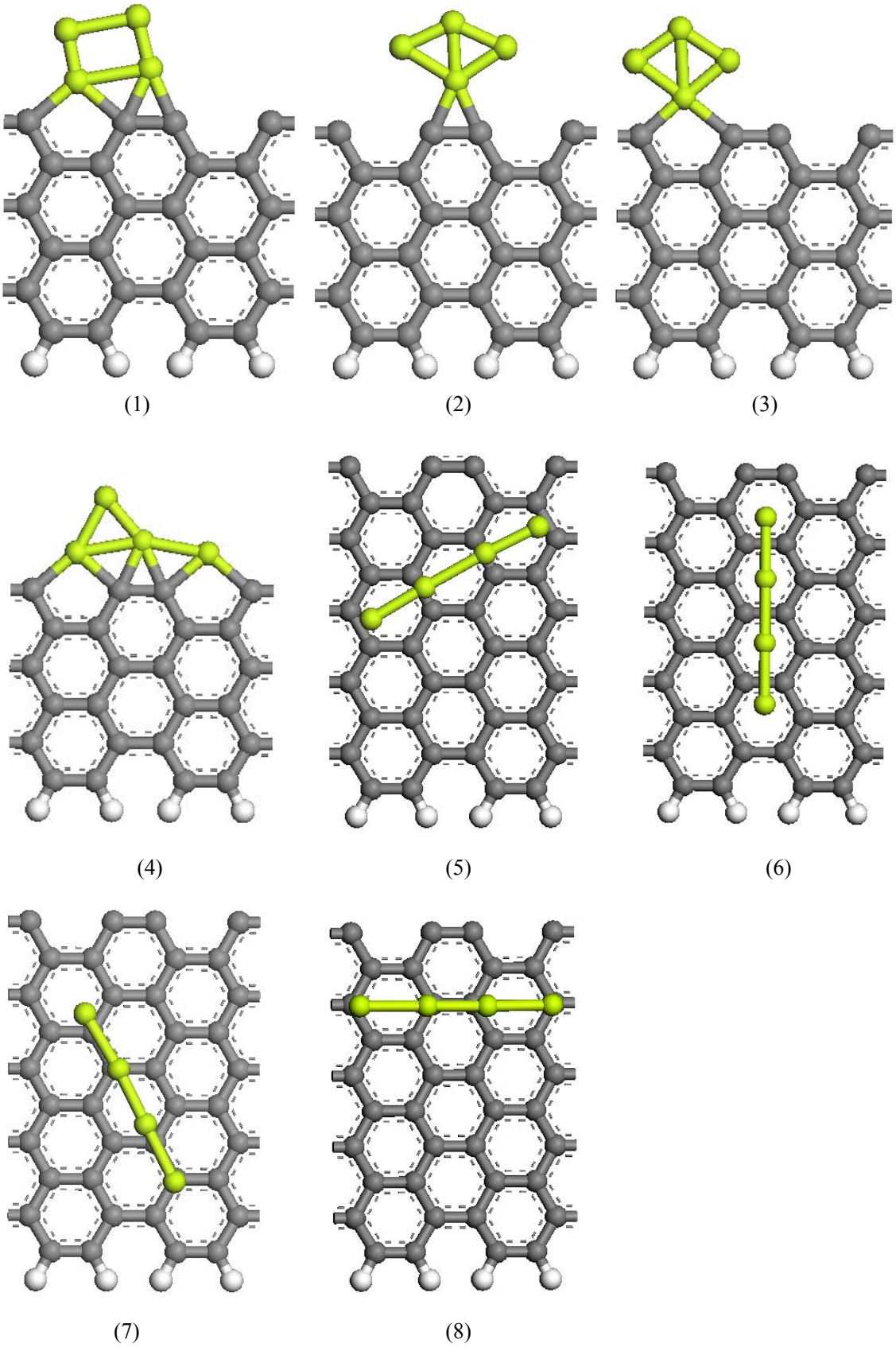
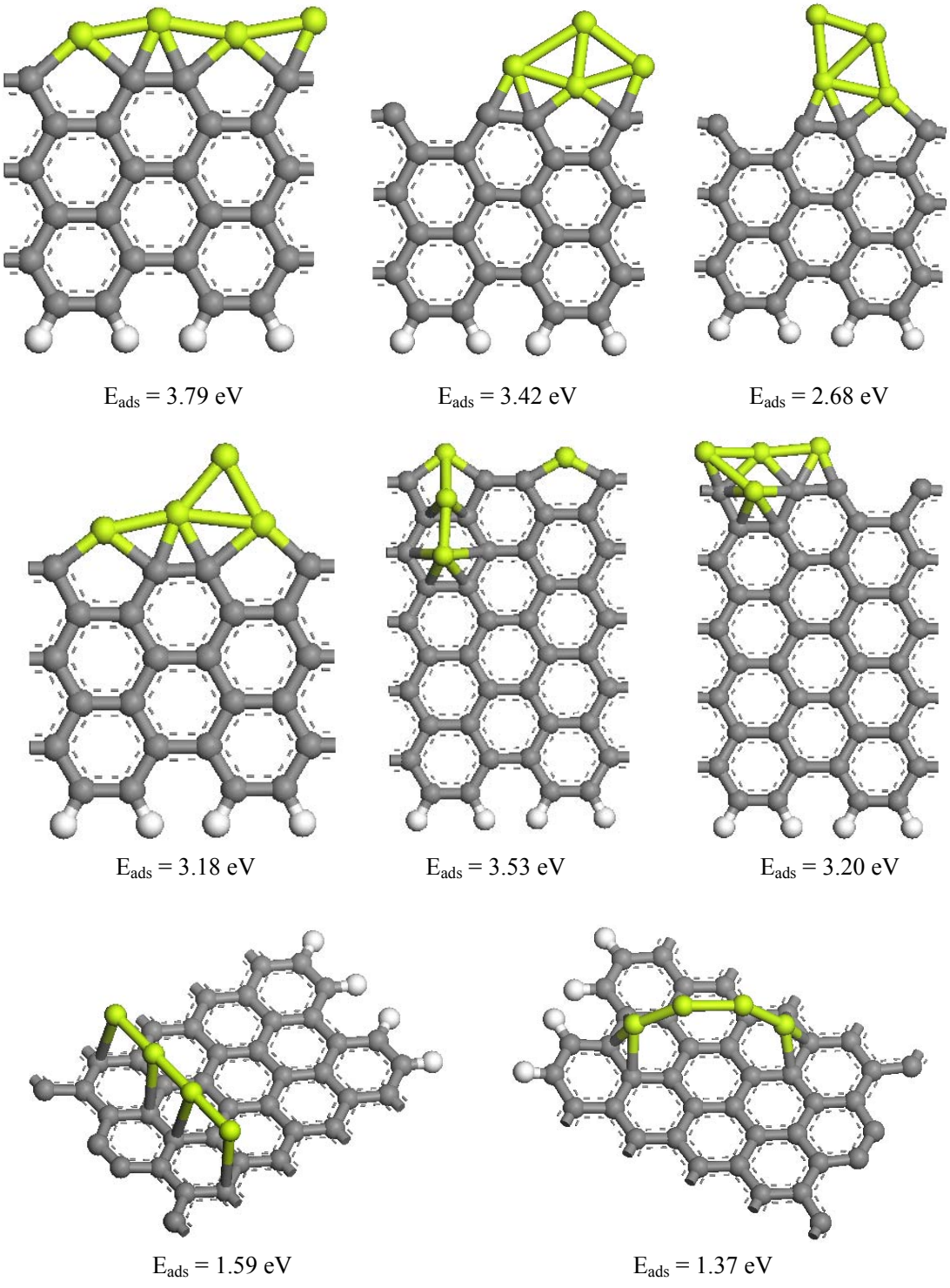


Figure S3. The final configurations for the adsorption of Be atoms on AGNR.



E_{ads} = 3.79 eV

E_{ads} = 3.42 eV

E_{ads} = 2.68 eV

E_{ads} = 3.18 eV

E_{ads} = 3.53 eV

E_{ads} = 3.20 eV

E_{ads} = 1.59 eV

E_{ads} = 1.37 eV

Figure S4. Various initial configurations for the adsorption of B atoms on AGNR.

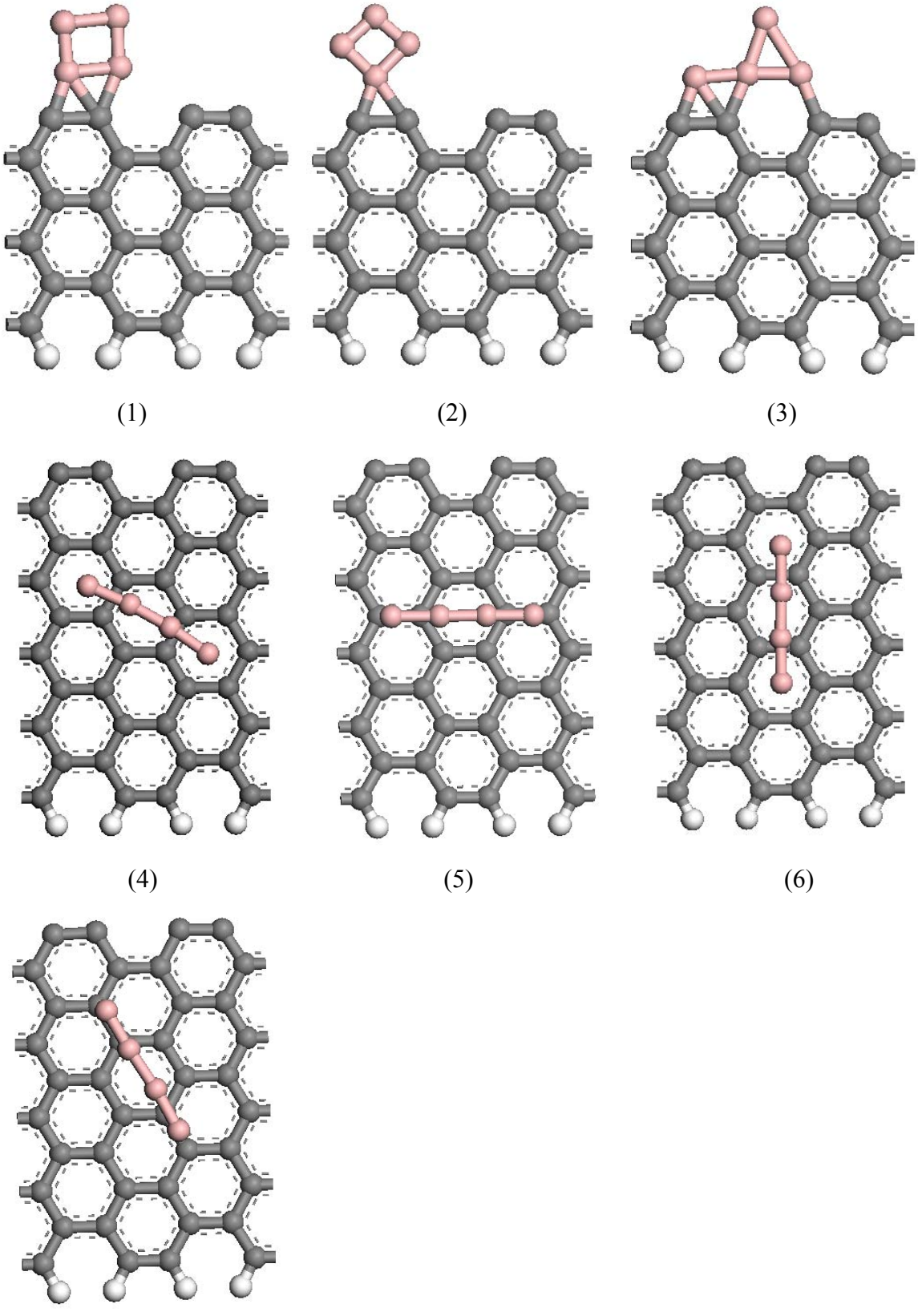
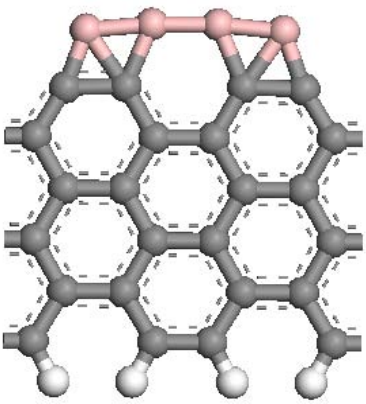
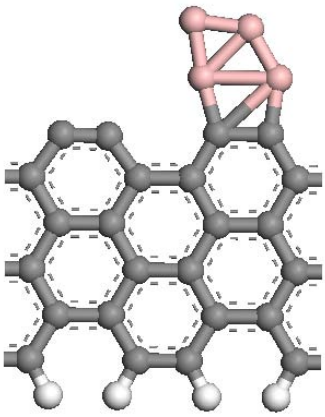


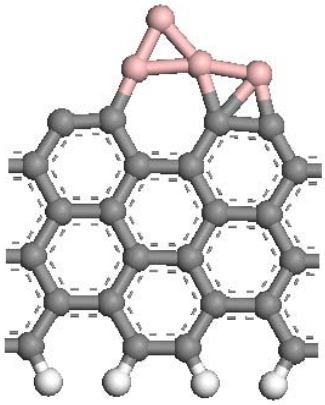
Figure S5. The final configurations for the adsorption of B atoms on AGNR.



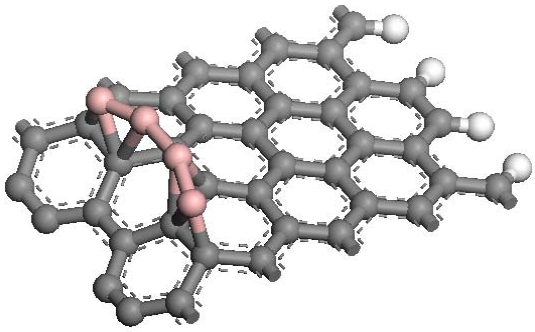
E_{ads} = 6.26 eV



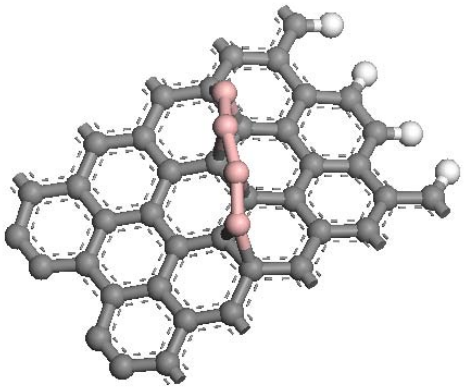
E_{ads} = 5.39 eV



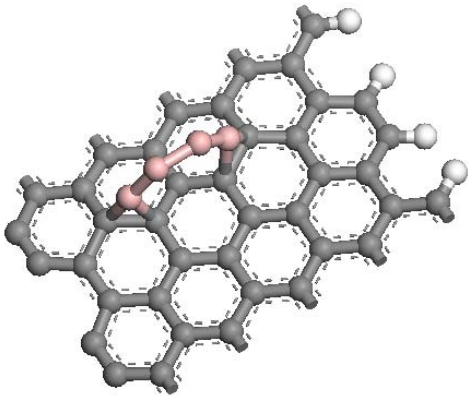
E_{ads} = 5.41 eV



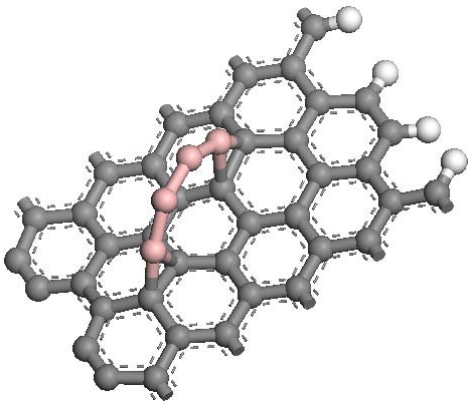
E_{ads} = 3.60 eV



E_{ads} = 3.51 eV

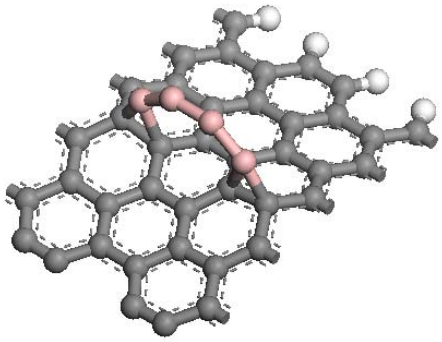


E_{ads} = 3.64 eV



E_{ads} = 3.69 eV

Figure S5 (Continued)



E_{ads} = 3.86 eV