Supplementary Information

Ab initio study of lithium decoration of popgraphene and hydrogen storage capacity of the hybrid nanostructure

P. Álvarez-Zapatero[a,*], A. Herrero[a], A. Lebon[b], L. J. Gallego[c], A. Vega[a]

[a] Departamento de Física Teórica, Atómica y Óptica, Universidad de Valladolid, E–47011 Valladolid, Spain
[b] Laboratoire de Chimie Électrochimie Moléculaire et Chimie Analytique, UEB/UBO, UMR CNRS 6521, 29238 Brest Cedex, France
[c] Departamento de Física de la Materia Condensada, Facultad de Física, Universidad de Santiago de Compostela, E–15782 Santiago de Compostela, Spain

[*]**Corresponding Author:**
Email: pablo.alvarez.zapatero@uva.es

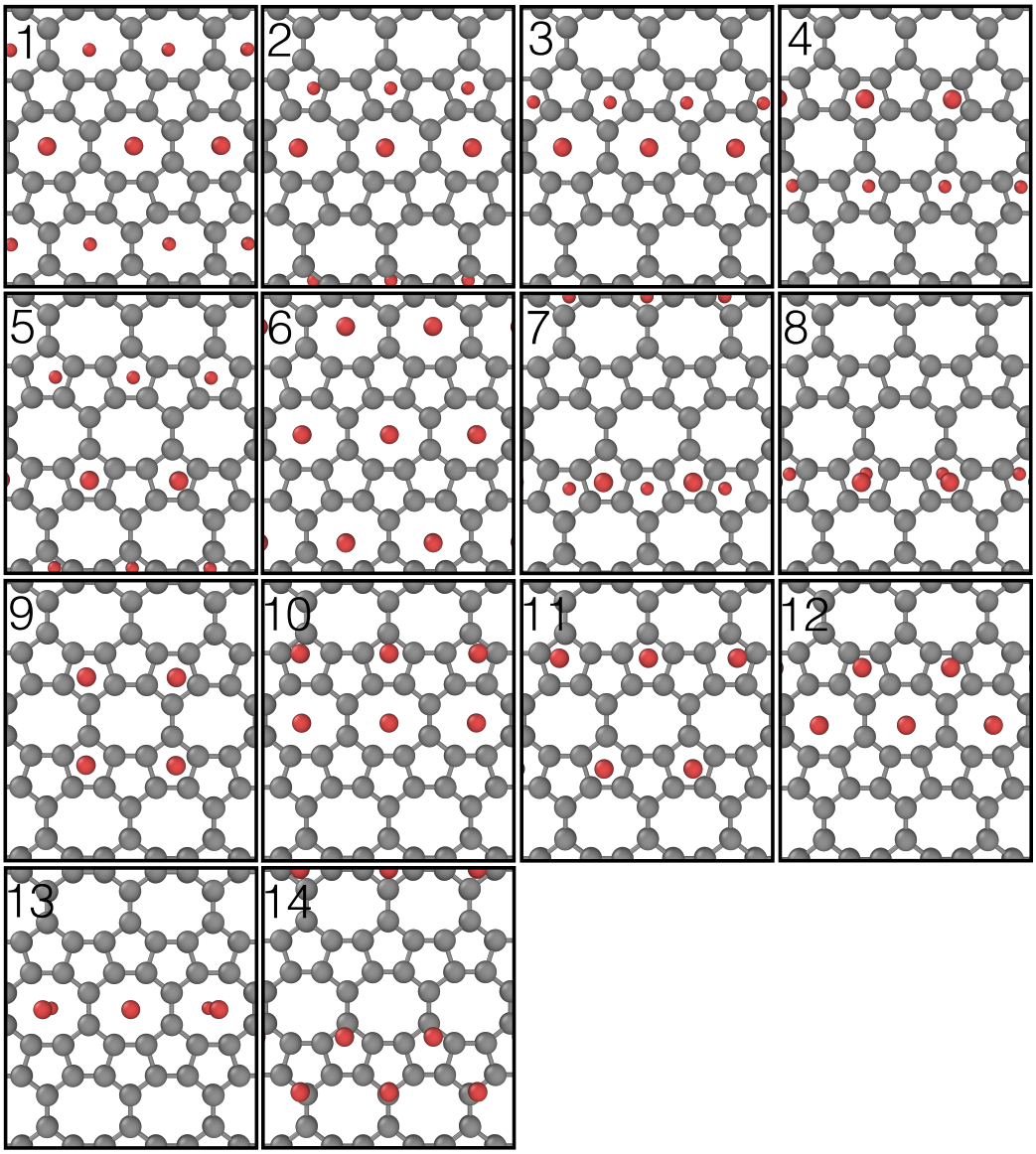

Fig. S1. Relaxed structures of popgraphene with two Li atoms adsorbed on different positions. The C and Li atoms are plotted as dark grey balls and red balls, respectively. The Li atoms on the front side have a greater size than the Li atoms on the rear side. The cohesive energies and formation energies are shown in Table S1.

Table S1. Cohesive energies and formation energies (in eV) of the structures shown in Fig. S1.

	Cohesive Energy	Formation Energy
1	6.873	1.983
2	6.868	1.945
3	6.864	1.918
4	6.863	1.908
5	6.861	1.897
6	6.860	1.890
7	6.860	1.889
8	6.859	1.880
9	6.858	1.875
10	6.855	1.854
11	6.854	1.850
12	6.852	1.834
13	6.847	1.800
14	6.841	1.760

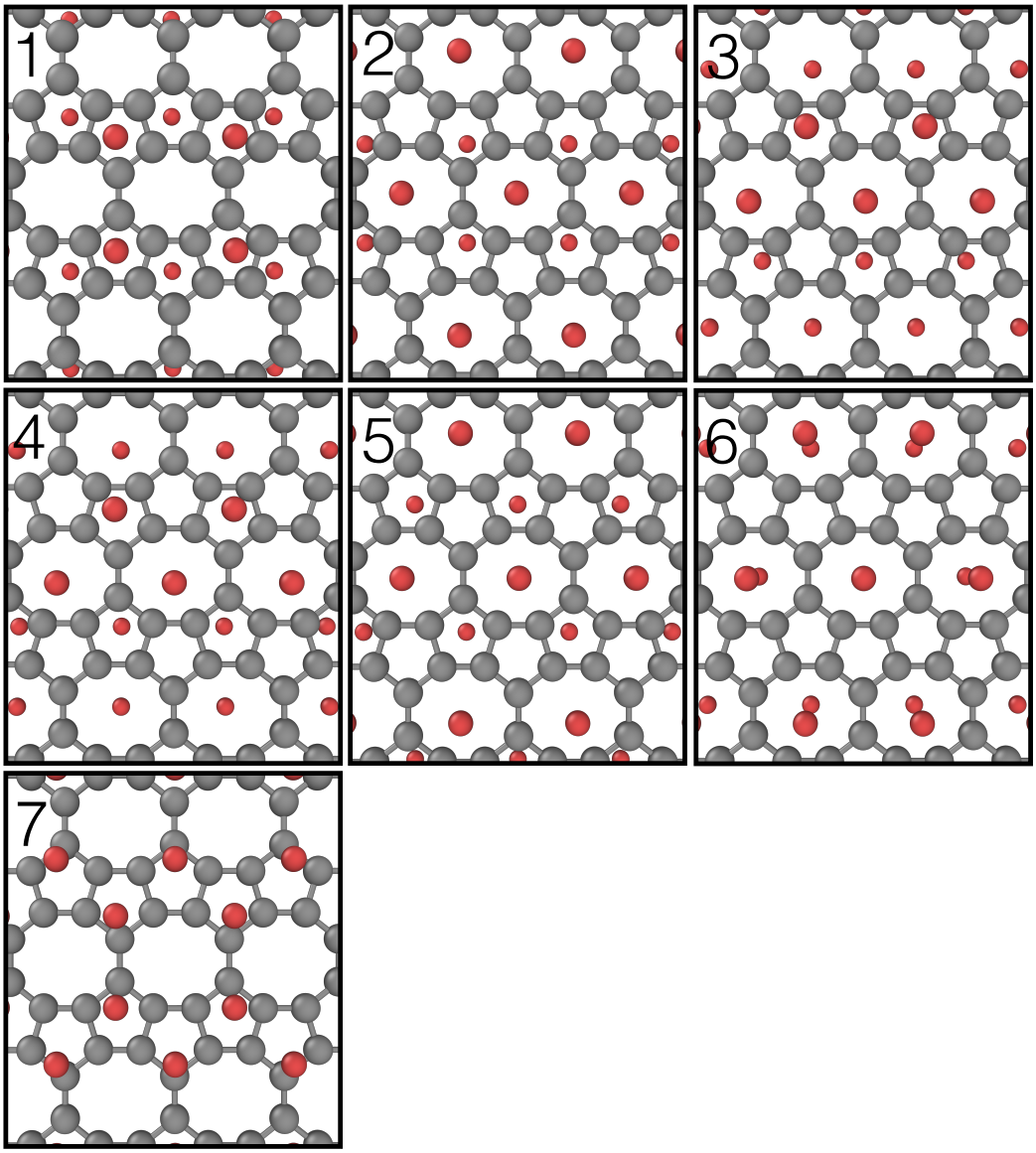

Fig. S2. Relaxed structures of popgraphene with four Li atoms adsorbed on different positions. The C and Li atoms are plotted as dark grey balls and red balls, respectively. The Li atoms on the front side have a greater size than the Li atoms on the rear side. The cohesive energies and formation energies are shown in Table S2.

Table S2. Cohesive energies and formation energies (in eV) of the structures shown in Fig. S2.

	Cohesive Energy	Formation Energy
1	-6.236	1.876
2	-6.220	1.814
3	-6.218	1.807
4	-6.218	1.806
5	-6.216	1.798
6	-6.190	1.696
7	-6.180	1.657

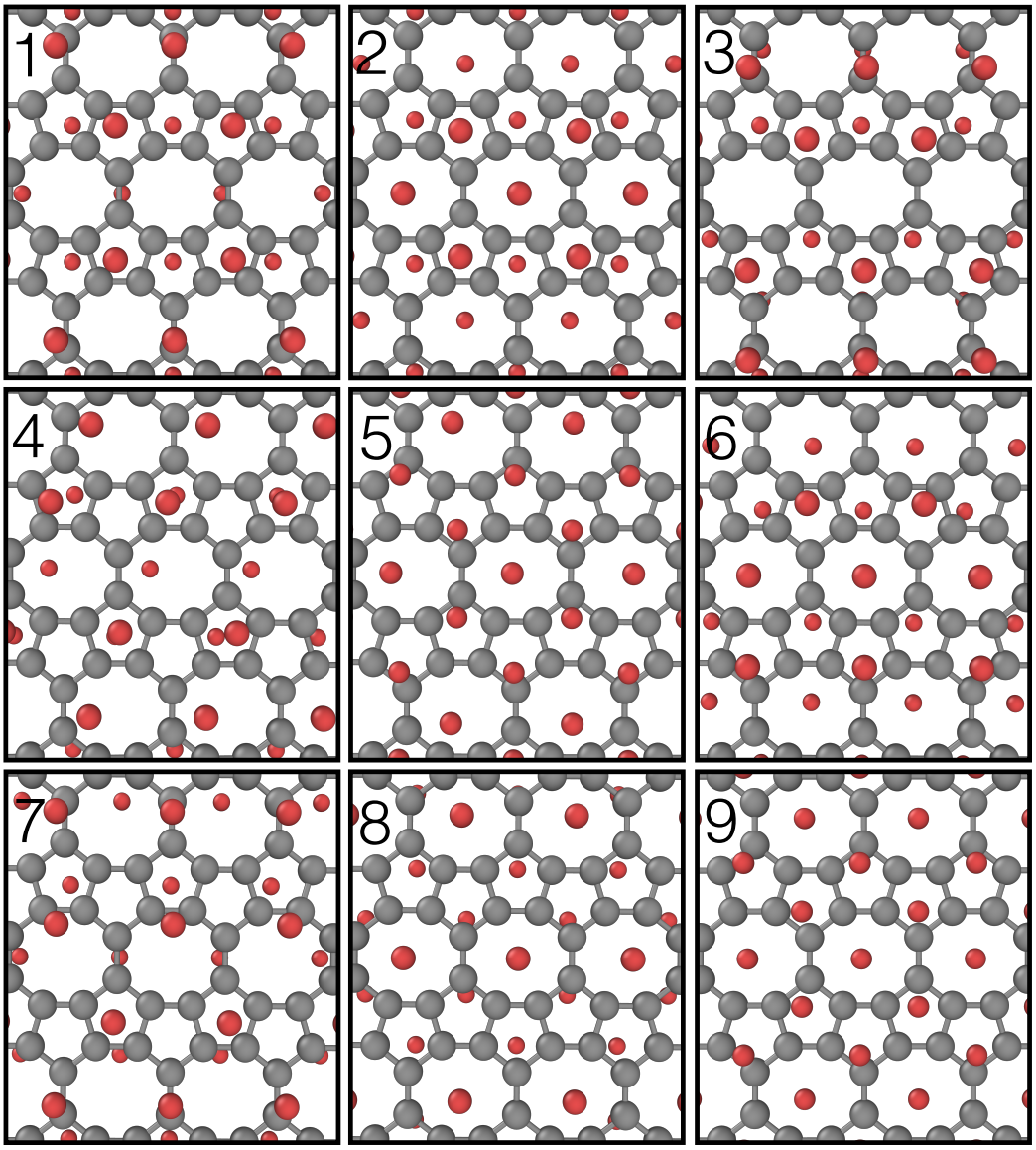

Fig. S3. Relaxed structures of popgraphene with six Li atoms adsorbed on different positions. The C and Li atoms are plotted as dark grey balls and red balls, respectively. The Li atoms on the front side have a greater size than the Li atoms on the rear side. The cohesive energies and formation energies are shown in Table S3.

Table S3. Cohesive energies and formation energies (in eV) of the structures shown in Fig. S3.

	Cohesive Energy	Formation Energy
1	5.718	1.779
2	5.706	1.741
3	5.705	1.739
4	5.698	1.718
5*	5.698	1.717
6	5.698	1.717
7	5.687	1.685
8	5.670	1.632
9**	5.645	1.558

* Structure of the right-hand panel of Fig. 3.
** Structure of the left-hand panel of Fig. 3.

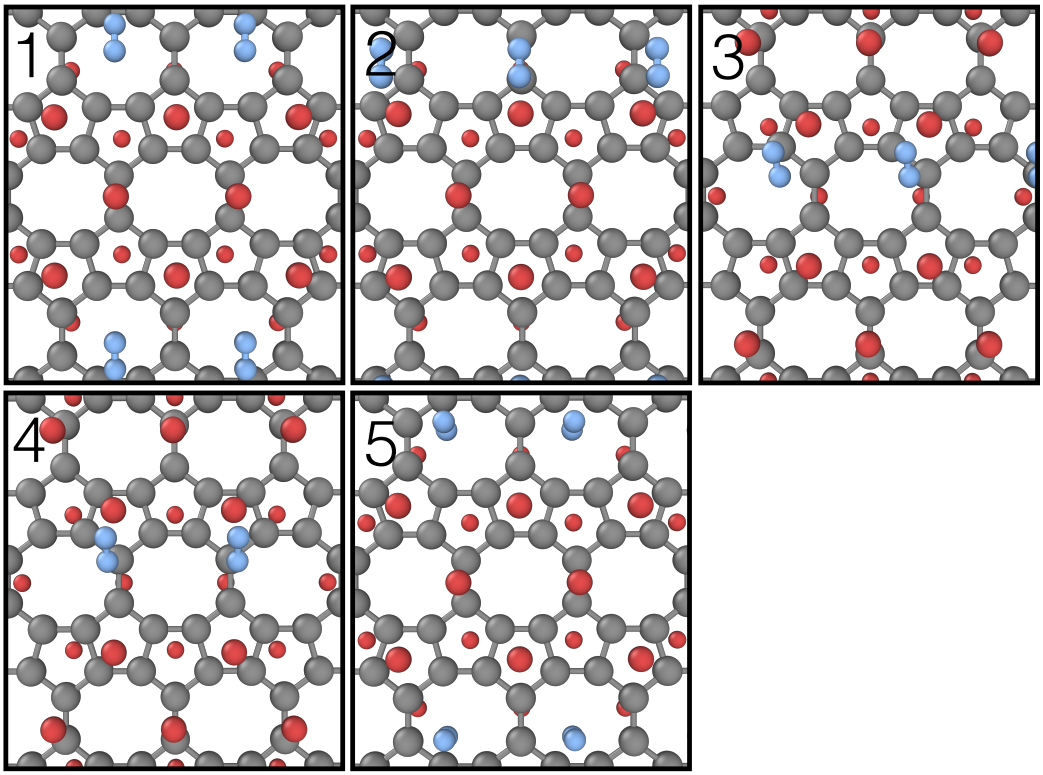

Fig. S4. Relaxed structures of the 6Li/PG + H_2 system. The H_2-adsorption energies are shown in Table S4. The C, Li and H atoms are plotted as dark grey balls, red balls and small light blue balls, respectively. The Li and H atoms on the front side have a greater size than the Li and H atoms on the rear side.

Table S4. H_2-adsorption energies (in eV) of the structures shown in Fig. S4.

	Adsorption Energy
1	0.155
2	0.151
3	0.151
4	0.151
5	0.136

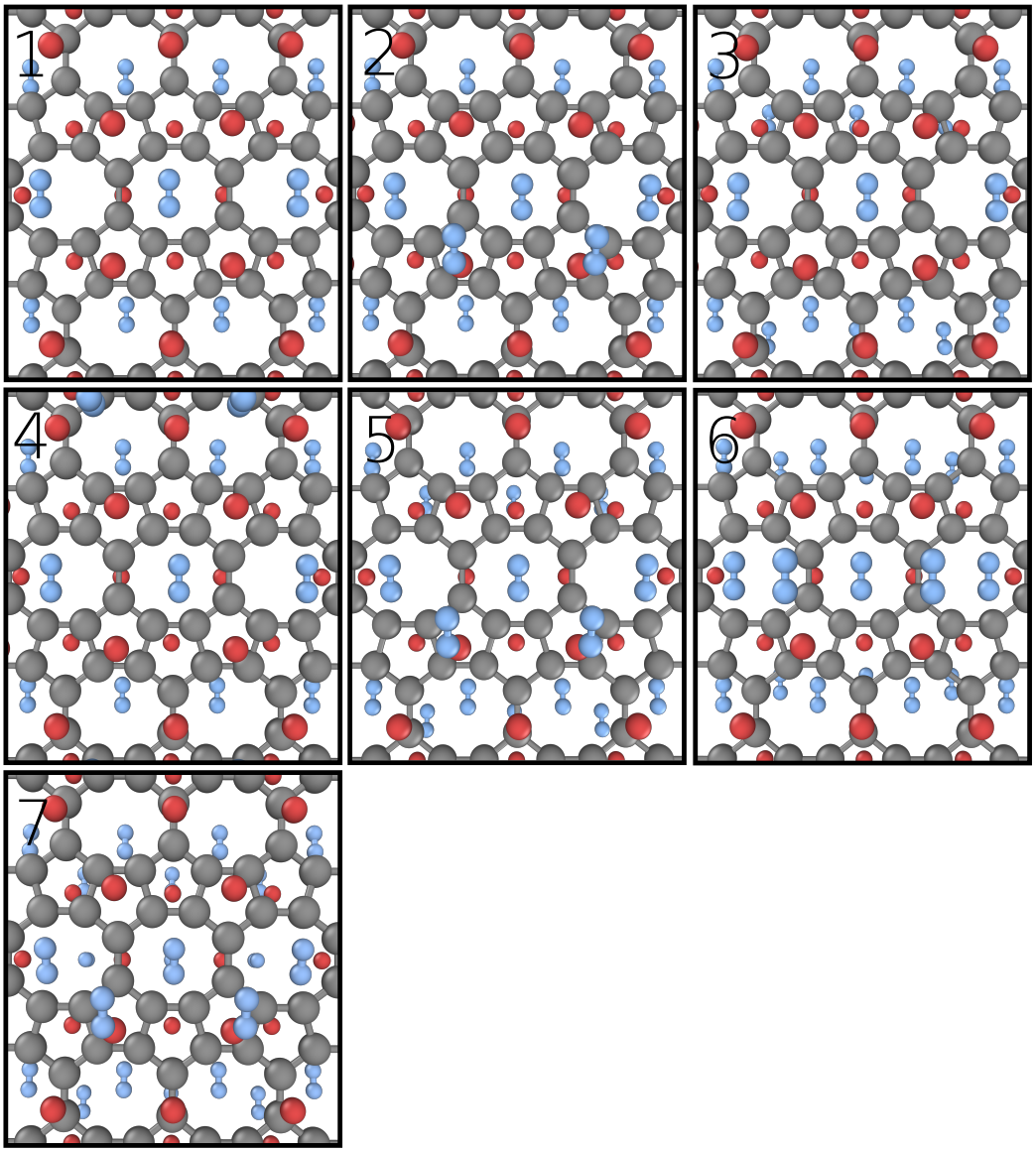

Fig. S5. Relaxed structures of the systems 6Li/PG + nH$_2$ (n = 2-5). The H$_2$-adsorption energies are shown in Table S5. The C, Li and H atoms are plotted as dark grey balls, red balls and small light blue balls, respectively. The Li and H atoms on the front side have a greater size than the Li and H atoms on the rear side.

Table S5. H_2-adsorption energies (in eV) of the structures shown in Fig. S5.

	n	Adsorption Energy
1	2	0.135
2	3	0.115
3	—	0.104
4	—	0.103
5	4	0.105
6	—	0.102
7	5	0.094