Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information: Lithium Storage on Carbon Nitride, Graphenylene and Inorganic Graphenylene

Marlies Hankel[*,†] and Debra J. Searles[†,‡]

Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, Brisbane, QLD 4072, Australia, and School of Chemistry and Molecular Bioscience, The University of Queensland, Brisbane, QLD 4072, Australia

E-mail: m.hankel@uq.edu.au

[*]To whom correspondence should be addressed
[†]AIBN, The University of Queensland
[‡]SCMB, The University of Queensland

K-point convergence

Convergence tests with different k-point meshes have been carried out. Initial lattice optimisations of the unit cell have been carried out with a 11 x 11 x 1 k-points mesh. Once lattice optimisation was achieved convergence test with respect to k-points have been carried out for the unit cell. It was found that a 3 x 3 x 1 k-points mesh is sufficient to converge the total energies. After this a 2 x 2 x 1 supercell was created and the convergence of the total energy was tested for different k-point meshes of 1 x 1 x 1, 3 x 3 x 1 and 5 x 5 x 1 k-points. It was found that a mesh of 3 x 3 x 1 k-points is sufficient. Li adsorption energies have been tested with different k-point meshes as well. Here we checked 1 x 1 x 1, 3 x 3 x 1 and 5 x 5 x 1 k-point meshes. Again, it was found that a 3 x 3 x 1 k-points mesh is sufficient to converge the Li adsorption energies. In fact for g-CN for example there is no difference in the total energies of the 2 x 2 x 1 supercell membrane and also in the adsorption energies for 1 Li in its preferred position when comparing the results for the 3 x 3 x 1 and the 5 x 5 x 1 k-point mesh.

Additional figures

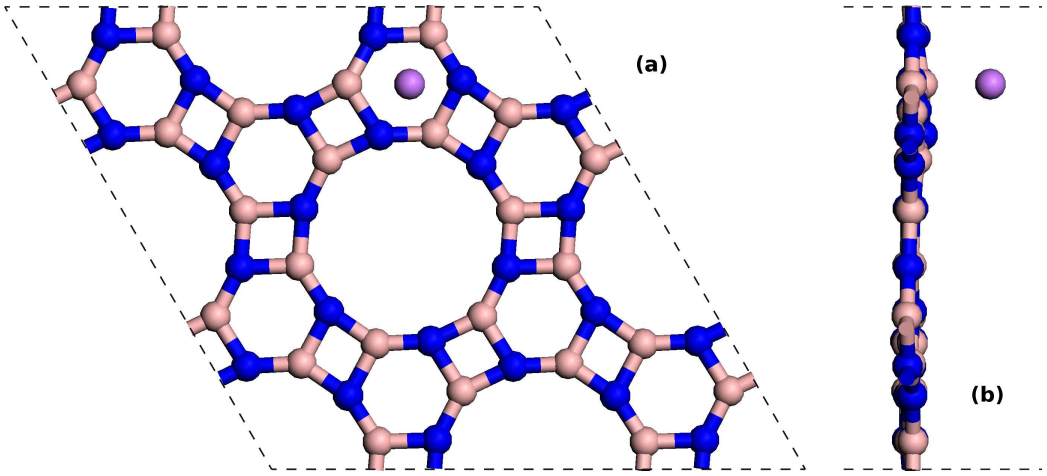

Figure S1: One lithium atom adsorbed over a ring on IGP. The pink balls represent boron, the blue balls nitrogen and the purple ball lithium.

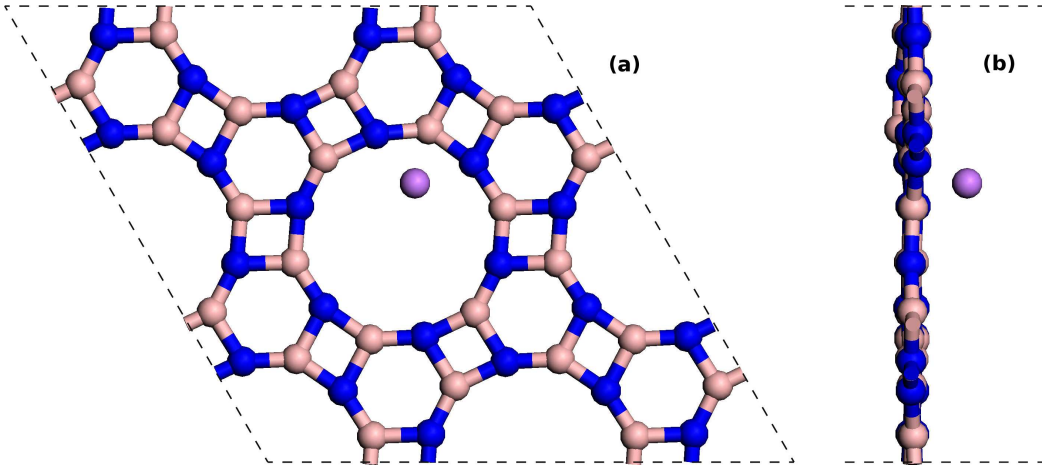

Figure S2: One lithium atom adsorbed over a pore on IGP. The pink balls represent boron, the blue balls nitrogen and the purple ball lithium.

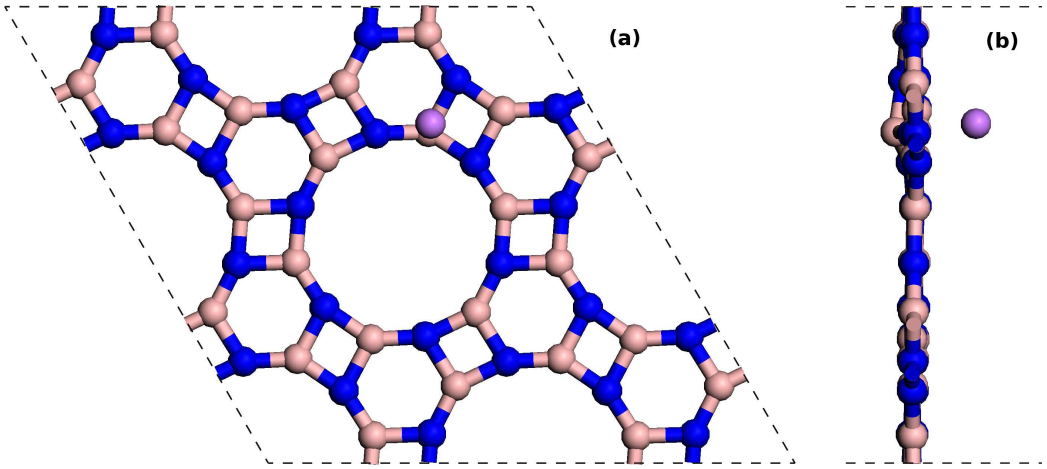

Figure S3: One lithium atom adsorbed over a boron atom on IGP. The pink balls represent boron, the blue balls nitrogen and the purple ball lithium.

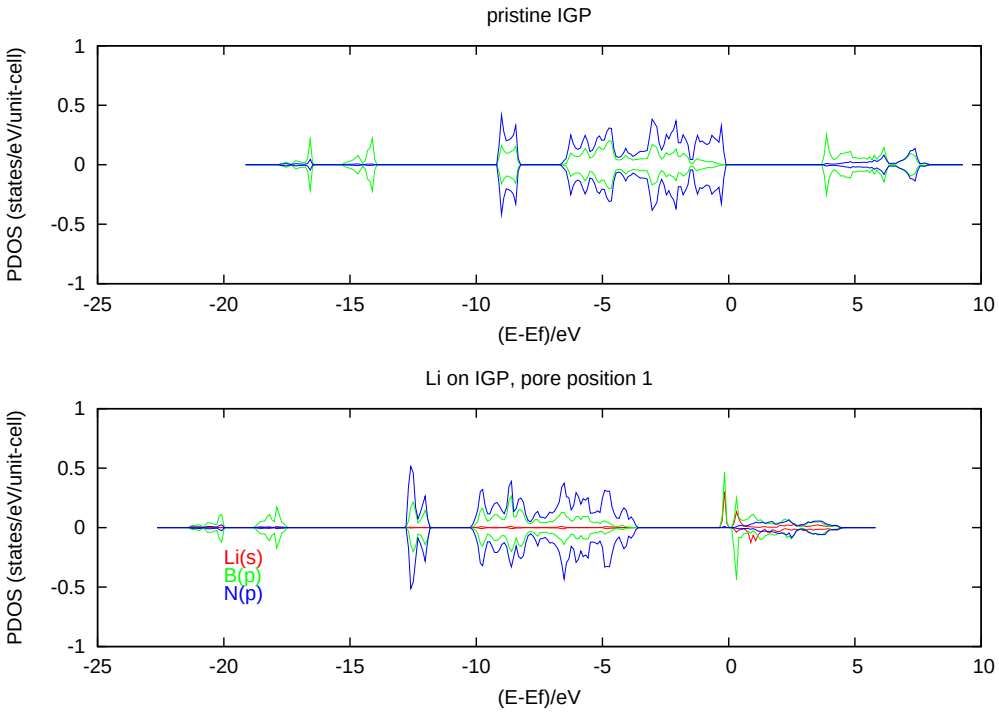

Figure S4: Partial density of states for pristine IGP (top panel) and Li adsorbed over the pore of IGP (bottom panel). For the latter the closest B and one of the N in close proximity were chosen.

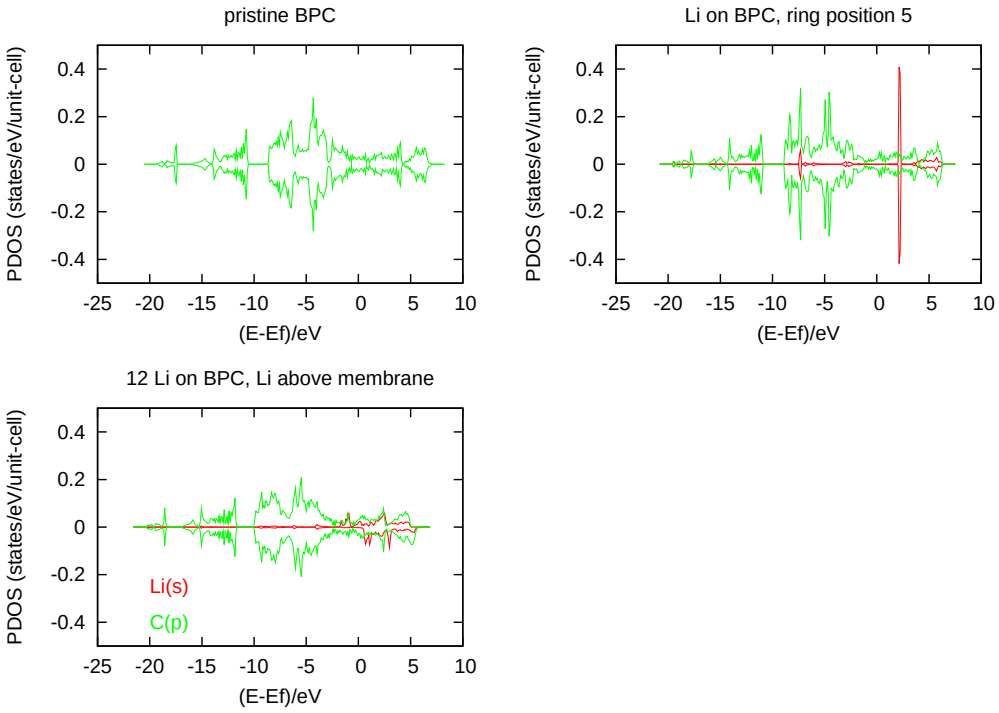

Figure S5: Partial density of states for pristine BPC (top left panel), Li adsorbed over a ring of BPC (top right panel) and 12 Li adsorbed all above the BPC membrane (bottom left panel). For the case of 12 Li one representative Li was chosen. In cases of 1 Li and 12 Li one representative C in close proximity was chosen.

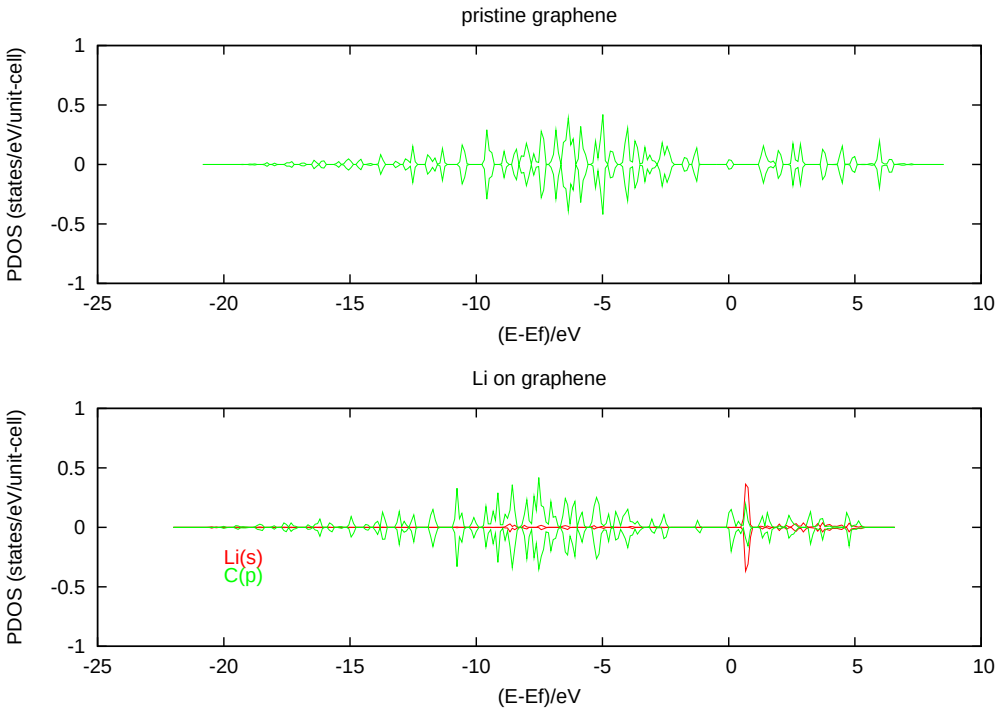

Figure S6: Partial density of states for pristine graphene (top panel) and Li adsorbed over one of the rings of graphene (bottom panel). For the latter, one representative C in close proximity was chosen.