Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting information for

Li diffusion through the doped and defected graphene

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1. NEB overestimates the energy barrier compared to Single point calculation with in 0.5-10 % error range.

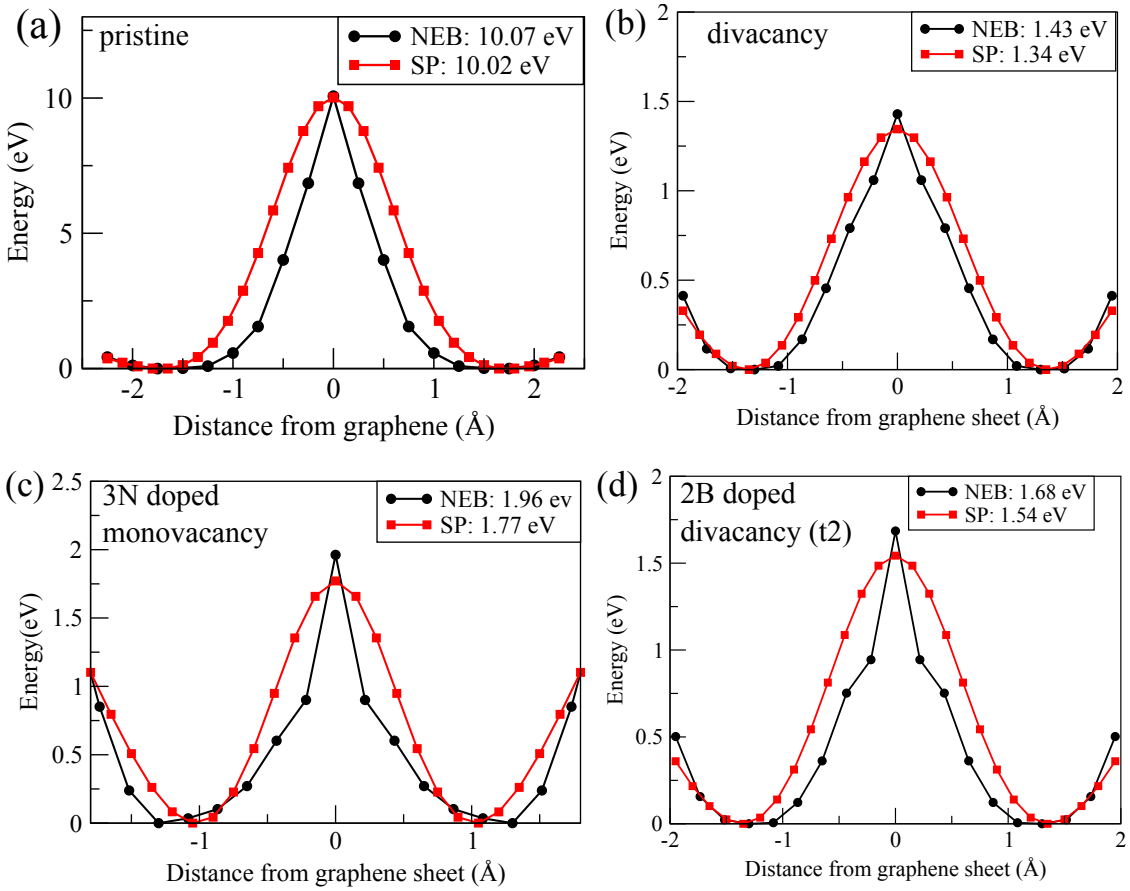

Figure S1: Comparison between single point calculation and nudged elastic band (NEB) method for (a) pristine graphene, (b) graphene with divacancy, (c) three nitrogen doped monovacancy and (d) two boron doped divacancy (type 2)

2. The PDOS peak of Li in the conduction band lies almost in the same position for B doped divacancy.

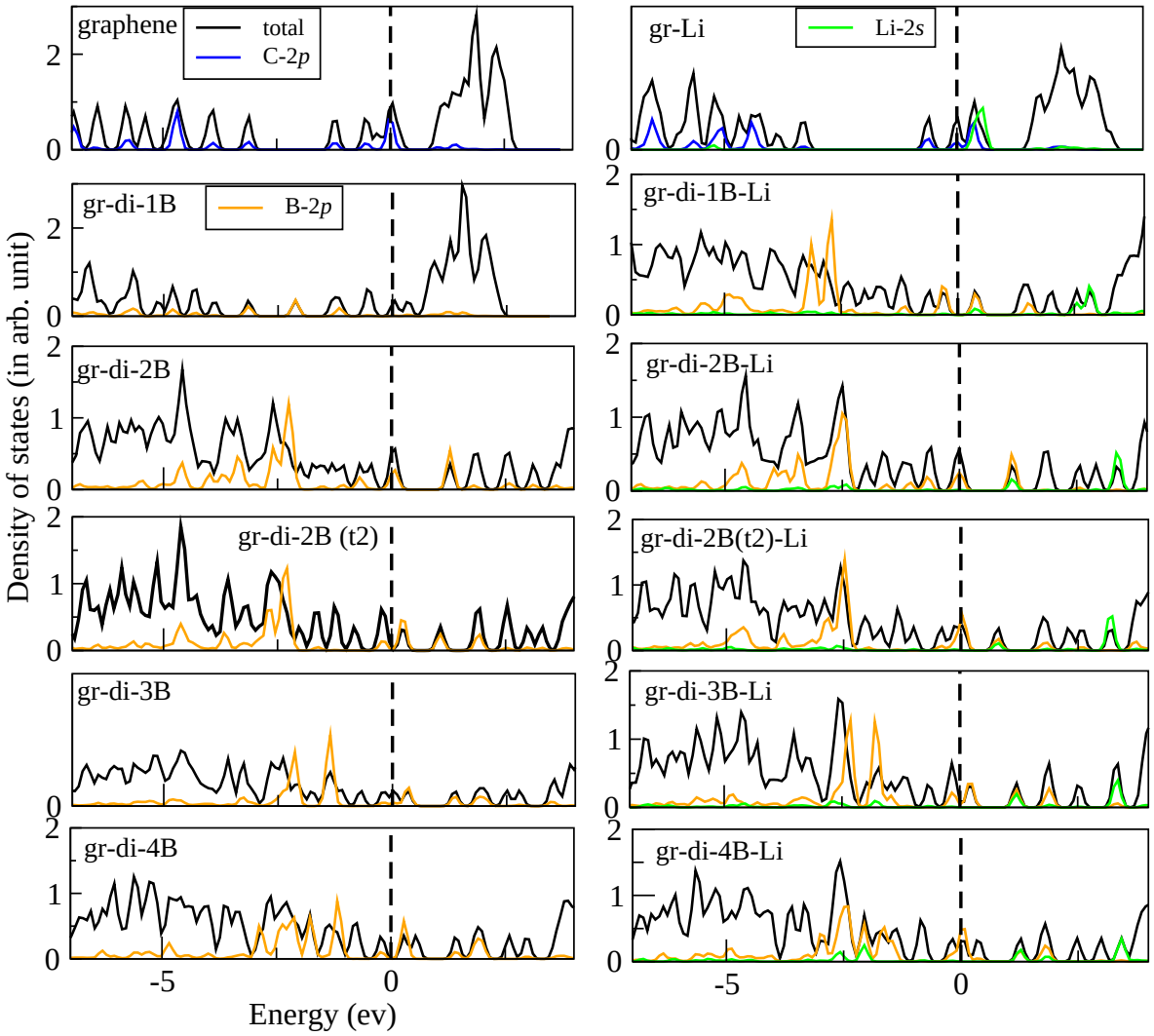

Figure S2: Density of states for pristine and B doped divacancy graphene in the (a) absence and (b) presence of Li

In the case of B doping, the PDOS peak of Li shifts to the higher energy value above the Fermi level indicating stronger Li adsorption energy compared to the pristine graphene case. The existence of this peak almost in the same position for all the B doped divacancy cases corresponds to consistently low energy barriers and better adsorption energies.