Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Ab initio study of sodium intercalation into disordered carbon

Ping-chun Tsai[a,b], Sai-Cheong Chung[a,c], Shih-kang Lin[b], and Atsuo Yamada[a,c,*]

Supporting information

a Department of Chemical System Engineering, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan;

b Department of Materials Science and Engineering, National Cheng Kung University, Tainan 70101, Taiwan

c Unit of Element Strategy Initiative for Catalysts & Batteries, ESICB, Kyoto University, Kyoto 615-8510, Japan

*yamada@chemsys.t.u-tokyo.ac.jp

Figures S1

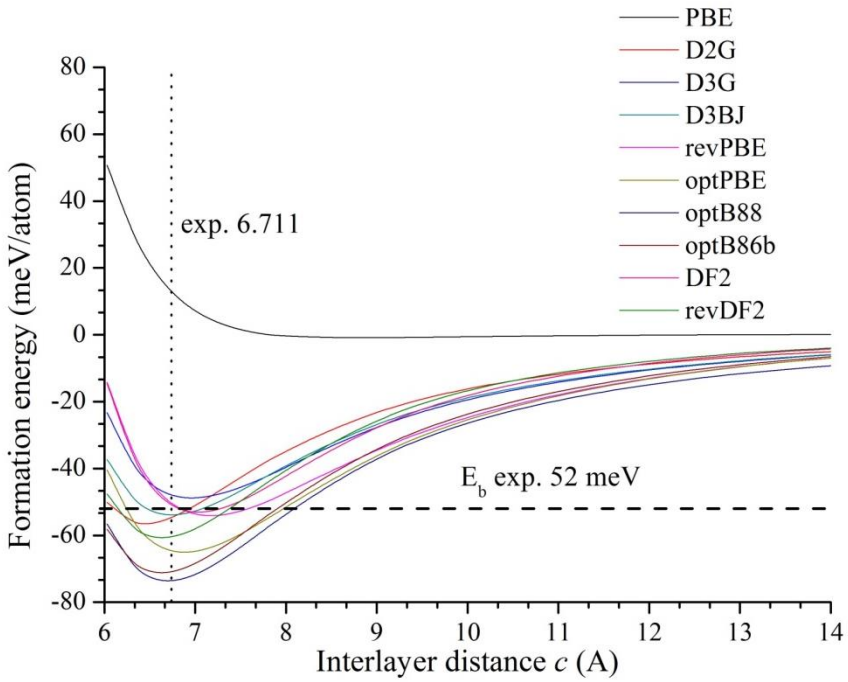

Figure S1 Formation energies of graphite as a function of interlayer distance c calculated by GGA and nine different vdW functionals, where the minimum binding energy defines the equilibrium interlayer spacing c.

The formation energy of graphite is calculated from the change in total energies of $E[graphene\ sheets]$ and $E[graphite]$.

Figures S2

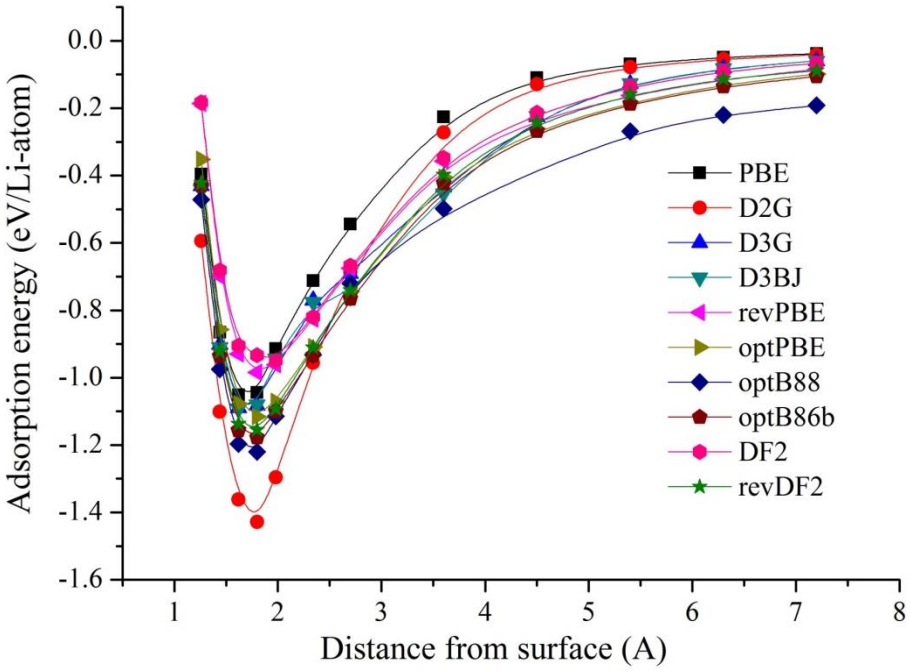

Figure S2 Adsorption energies of Li as a function of distance from the graphene sheet calculated by GGA and nine different vdW functionals.

The adsorption energy (E_{ab}) is defined to describe the stability of the adatom on hollow site of the surface according to the equation (2)

$$E_{ab} = E_{Li-surf} - E_{surf} - E_{Li} \quad (2)$$

where $E_{Li-surf}$, E_{surf}, and E_{Li} are the total energies of the Li adatom adsorbed on the surface of graphene, the free surface of graphene, and the isolated Li atom.

Figure S3

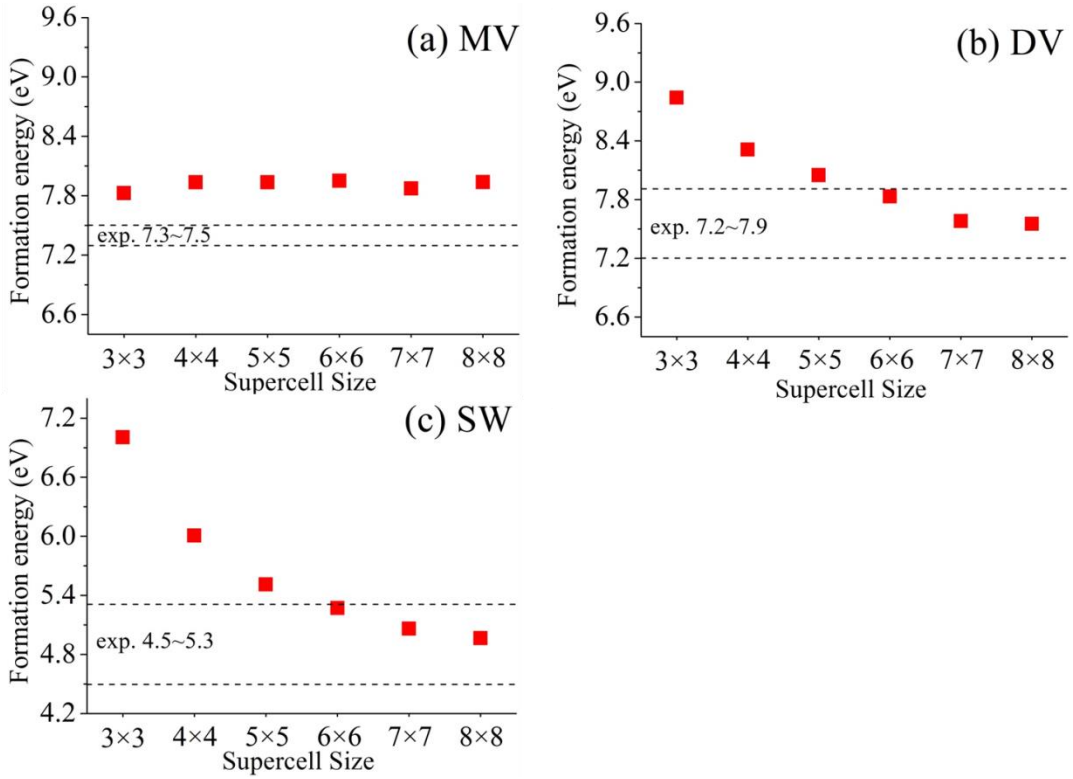

Figure S3 Defect formation energies of MV, DV, and SW point defects from 3 x 3 to 8 x 8 supercell sizes of graphene.

Table S1

Charge transfer (e) from Na^+ ions to graphene sheet and vertical distances (Å) between Na^+ ion and the graphene sheet for Na adsorption on a graphene sheet and intercalation into layer between graphene sheets. Only the values for the most stable sites in each case are shown.

	Pristine	Mono-vacancy	Di-vacancy	Stone-Wales
Adsorption	0.863 e / 2.13 Å	0.983 e / 2.08 Å	0.989 e / 1.90 Å	0.992 e / 2.09 Å
Intercalation	0.985 e / 1.98 Å	0.985 e / 1.81 Å	0.988 e / 1.63 Å	0.986 e / 1.88 Å