Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information for

Theoretical and experimental investigations of the Li storage capacity in single-walled carbon nanotube bundles

G. Ramos-Sanchez[1], G. Chen[2], A. R. Harutyunyan[2], and P. B. Balbuena[1*]
[1]Department of Chemical Engineering, Texas A&M University, College Station, TX, 77843,
[2]Honda Research Institute USA Inc., Columbus, OH, 43212
***e-mail: balbuena@tamu.edu**

a) Final intercalation structures in a bundle at fixed density

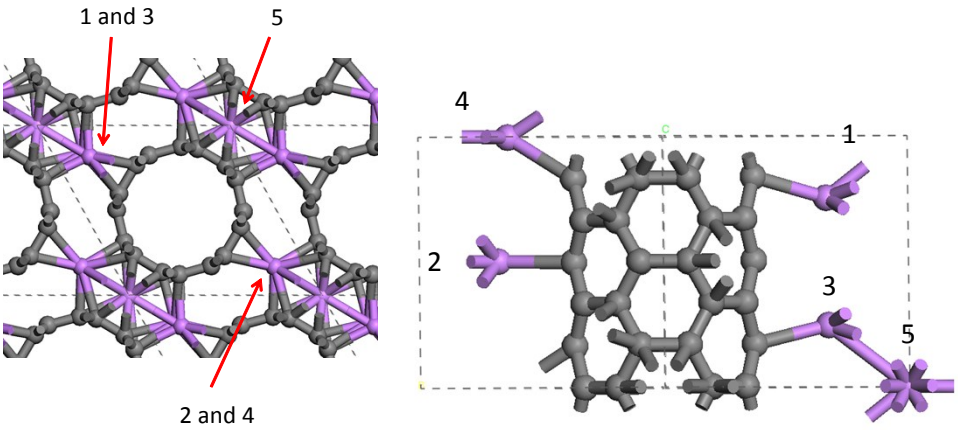


Figure S1. Intercalation in SWCNT (4,4) at fixed density (intercalation capacity shown in Figure 3a)

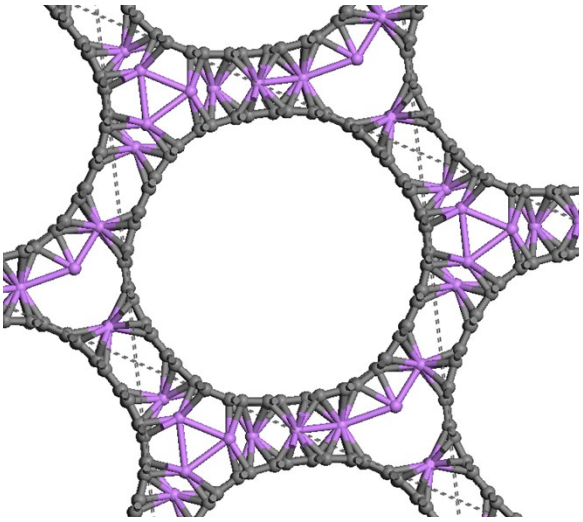


Figure S2. Intercalation in SWCNT (12,12) at fixed density (intercalation capacity shown in Figure 3b)

b) Model of SWCNT surface at fixed density

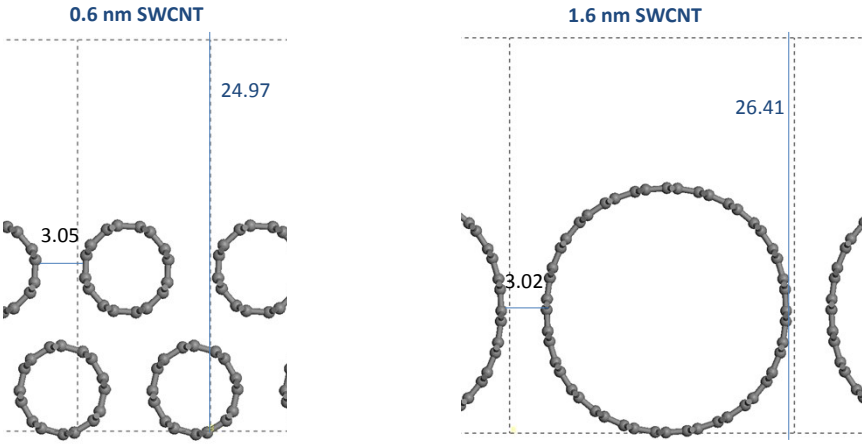
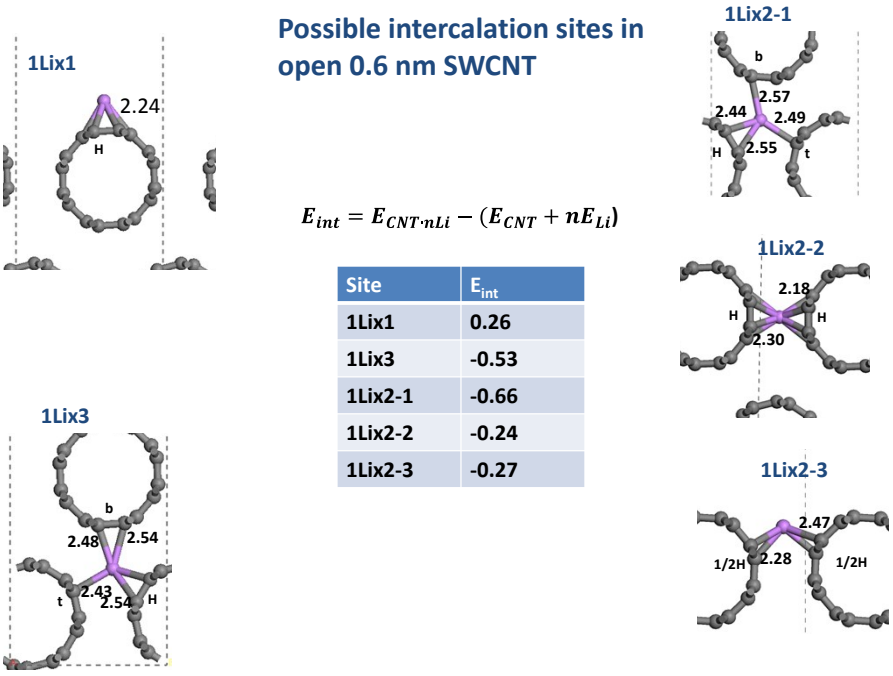
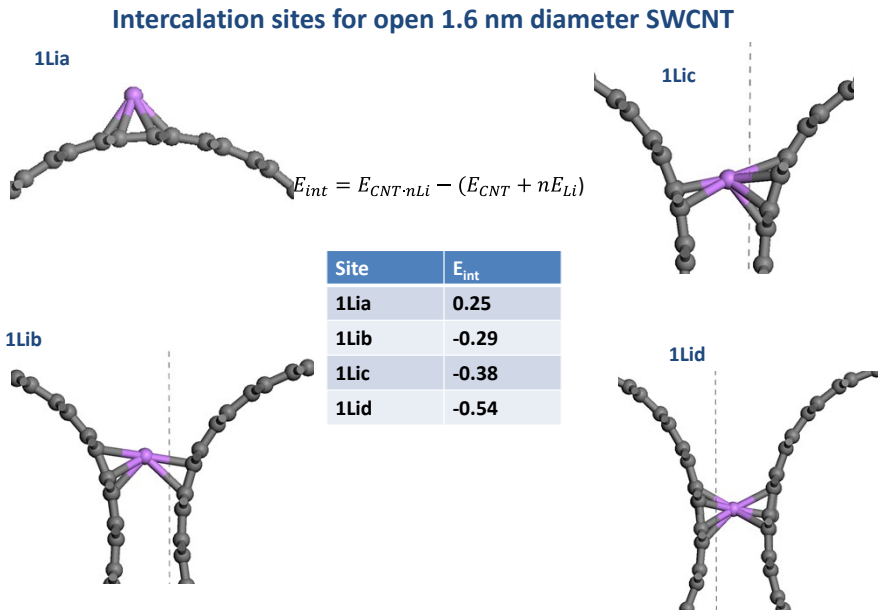


Figure S3. Models used to evaluate Li intercalation in (4,4) and (12,12) open nanotubes.



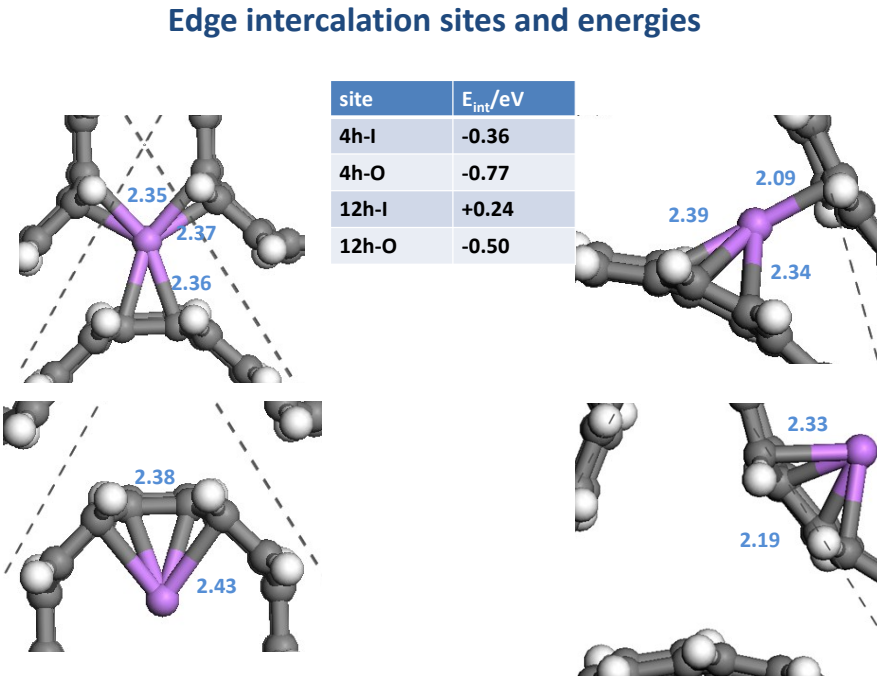
Site	E_{int}
1Lix1	0.26
1Lix3	-0.53
1Lix2-1	-0.66
1Lix2-2	-0.24
1Lix2-3	-0.27

Figure S4. Li intercalation sites and energies in (4,4) open nanotubes.



Site	E_{int}
1Lia	0.25
1Lib	-0.29
1Lic	-0.38
1Lid	-0.54

Figure S5. Li intercalation sites and energies in (12,12) open nanotubes.



site	E_{int}/eV
4h-I	-0.36
4h-O	-0.77
12h-I	+0.24
12h-O	-0.50

Figure S6. Li intercalation sites and energies in (4,4) (left) and (12,12) (right) open nanotubes terminated by H atoms. The nomenclature h-I is used for intercalation inside and h-O for intercalation outside of the nanotube.