SUPPORTING INFORMATION

Li-Functionalized Carbon Nanotubes for Hydrogen Storage: Importance of Size Effects

Ekaterina Anikina[†,‡], Amitava Banerjee[*,⊥], Valery Beskachko[‡], Rajeev Ahuja [†,⊥]

[†] Materials Theory Division, Department of Physics and Astronomy, Uppsala University, Box 516, 75120, Sweden

[‡] Institute of Natural Sciences and Mathematics, South Ural State University, 76, Lenin Prospekt, Chelyabinsk 454080, Russia

[⊥]Applied Materials Physics, Department of Materials and Engineering, KTH Royal Institute of Technology, S-100 44 Stockholm, Sweden

Corresponding Author:

*(AB) E-mail: amitava245@gmail.com

Supplementary figures

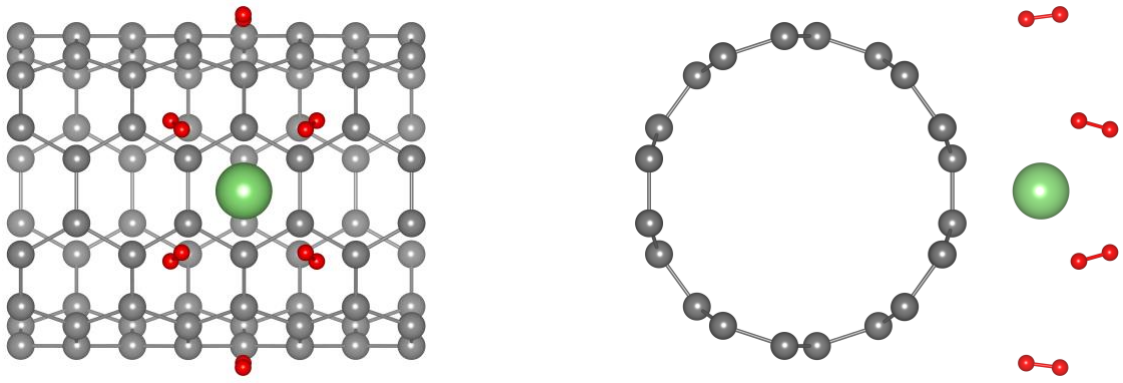

Figure S1. Configuration S+2 of the complex CNT(5,5)@ Li+6H_2 (external sorption, $N_c = 4$). C, Li, and H atoms are gray, green, and red, respectively.

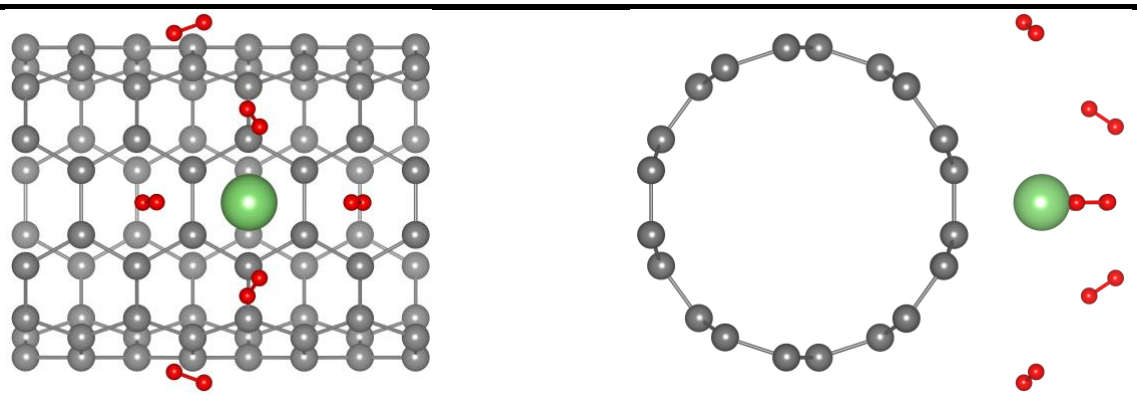

Figure S2. Configuration R+2 of the complex CNT (5,5)@Li+6H_2 (external sorption, N_c=4). C, Li, and H atoms are gray, green, and red, respectively.

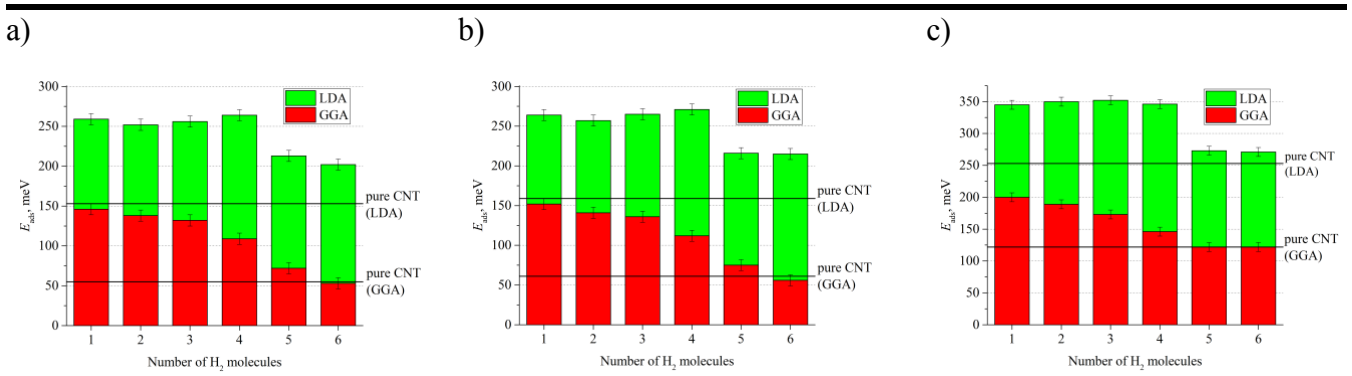

Figure S3. Hydrogen adsorption energies in the case of (a) external sorption on CNT(7,7)@Li; (b) external sorption on CNT(9,9)@Li; (c) internal sorption on CNT(9,9)@Li. GGA and LDA results are noted by red and green color, respectively. Adsorption energies on pure CNTs are noted by solid lines (for both GGA and LDA calclations).

Supplementary tables

Table S1. E_{bind} (meV) of H_2 Molecule in Complexes CNT(7,7)+kH_2 and CNT(7,7)@Li+kH_2 Calculated in GGA, DFT-D2, and LDA

k	CNT(7,7)@Li						CNT(7,7)					
	external surface			internal surface			external surface			internal surface		
	GGA	DFT-D2	LDA	GGA	DFT-D2	LDA	GGA	DFT-D2	LDA	GGA	DFT-D2	LDA
1	146	269	259	218	393	379	55	114	153	140	252	287
2	143	264	252	204	378	386	–	–	–	–	–	–
3	126	247	256	189	370	373	–	–	–	–	–	–
4	85	203	264	155	282	367	–	–	–	–	–	–