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双空位缺陷双层石墨烯储钠性能的第一性原理研究

杨绍斌[1,*] 李思南[2] 沈 丁[1] 唐树伟[3] 孙 闻[1] 陈跃辉[4]

([1]辽宁工程技术大学材料科学与工程学院，辽宁阜新 123000；[2]辽宁工程技术大学矿业学院，辽宁阜新 123000；[3]东北师范大学化学学院，长春 130024；[4]辽宁工程技术大学理学院，辽宁阜新 123000)

First-Principles Study of Na Storage in Bilayer Graphene with Double Vacancy Defects

YANG Shao-Bin[1,*] LI Si-Nan[2] SHEN Ding[1] TANG Shu-Wei[3] SUN Wen[1] CHEN Yue-Hui[4]

([1]*College of Materials Science and Engineering, Liaoning Technical University, Fuxin 123000, Liaoning Province, P. R. China*; [2]*College of Mining, Liaoning Technical University, Fuxin 123000, Liaoning Province, P. R. China*; [3]*Faculty of Chemistry, Northeast Normal University, Changchun 130024, P. R. China*; [4]*College of Science, Liaoning Technical University, Fuxin 123000, Liaoning Province, P. R. China*)

[*]Corresponding author. Email: lgdysb@163.com.

表 S1 自旋和非自旋态的 Na-双空位缺陷双层石墨烯体系的总能量 E_{total} 和平均层间距 $D_{g\text{-}g}$

Table S1 Total energies and average interlayer distances ($D_{g\text{-}g}$) between graphene layers for Na-double-vacancy defective bilayer graphene structures.

		4 × 4 super cell C_{62}				3 × 3 super cell C_{34}			
		AB	AB100	AB010	AB001	AB	AB100	AB010	AB001
E_{total}/eV	Spin	-9612.341	-10917.571	-10917.556	-10916.667	-5266.787	-6572.187	-6572.382	-6570.953
	Non-spin	-9612.345	-10917.574	-10917.557	-10916.671	-5266.787	-6572.165	-6572.369	-6570.948
$D_{g\text{-}g}$/nm	Spin	0.3280	0.3268	0.3812	0.3242	0.3394	0.3251	0.4071	0.3226
	Non-spin	0.3280	0.3268	0.3812	0.3242	0.3394	0.3251	0.4071	0.3290

表 S2 双层石墨烯平均层间距($D_{g\text{-}g}$)、C-C 键距($D_{C\text{-}C}$)和结合能(E_b)

Table S2 Average interlayer distances ($D_{g\text{-}g}$) between graphene layers, maximum distances between carbon atoms ($D_{C\text{-}C}$) and interlayer binding energies (E_b) for bilayer grapheme

	Stacking	C_{64} (4 × 4 supercell)			C_{36} (3 × 3 supercell)			
		GGA-PBE	Grimme	TS	GGA-PBE	Grimme	TS	Others
$D_{g\text{-}g}$/nm	AB	0.3840	0.3243	0.3318	0.3975	0.3255	0.3364	0.324[a],0.3482[b]
	AA	0.3601	0.3499	0.3514	0.3767	0.3758	0.3525	0.359[c], 0.355[d]
$D_{C\text{-}C}$/nm	AB	0.1421	0.1421	0.1421	0.1421	0.1420	0.1420	0.142[a], 0.143[b]
	AA	0.1421	0.1420	0.1420	0.1421	0.1421	0.1421	0.141[c]
E_b/(meV atom^{-1})	AB	-0.20	-26.22	-37.15	5.52	-20.34	-30.81	-50.6[e], -20.3[f]
	AA	4.82	-19.93	-31.22	3.12	-17.08	-24.81	-31.1[e], -10.4[f]

[a] vdW implemented in the VASP, Ref.1; [b] GGA-PBE based on SIESTA code, Ref.2; [c] LDA implemented in the VASP, Ref.3; [d] Experimental, Ref.4; [e] DFT-D functional, Ref.5; [f] vdW-DF functional, Ref.5

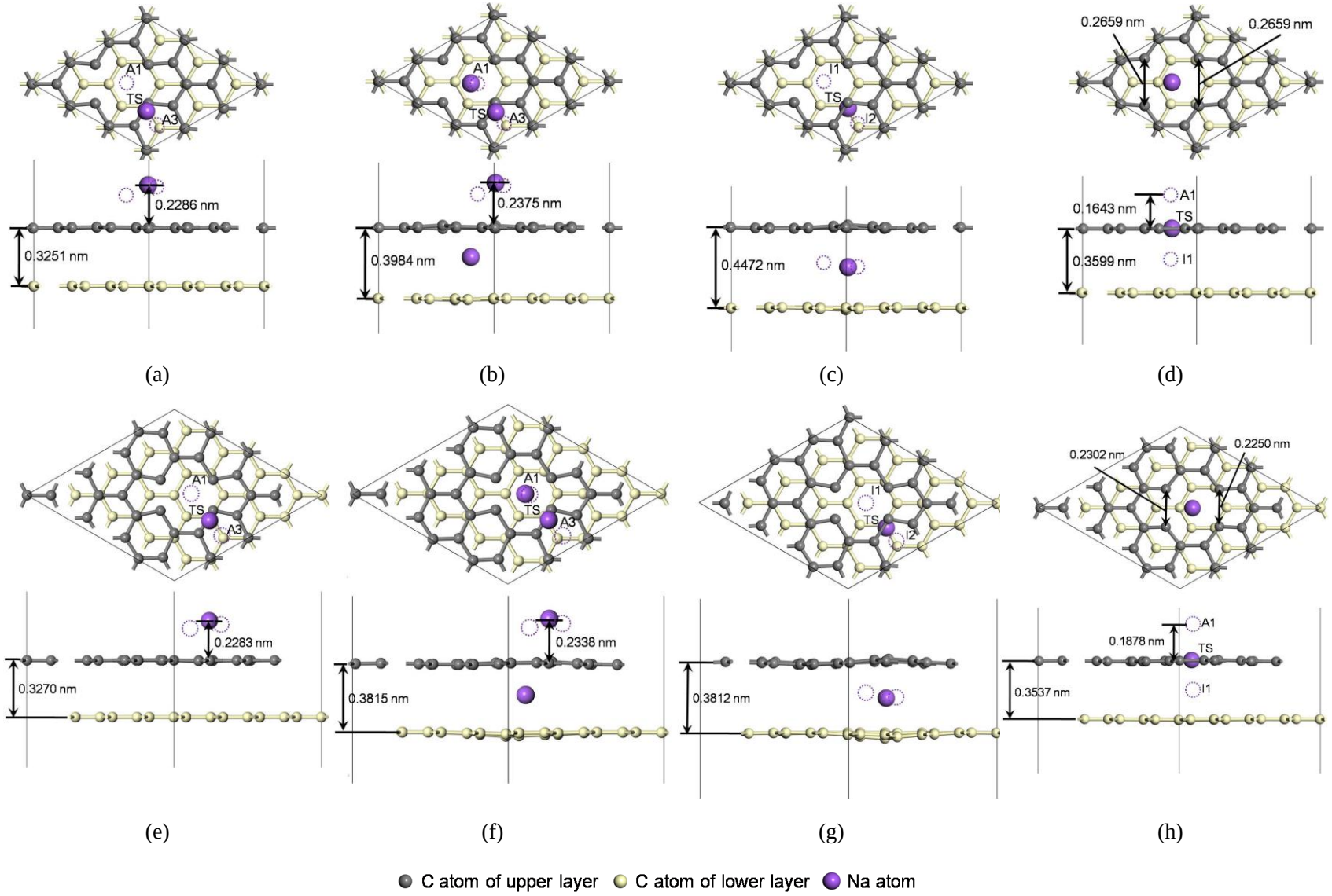

图 S1　Na 在 C_{34} 和 C_{62} 中沿不同路径扩散的过渡态(TS)结构

Fig.S1　Transition states (TS) for different Na diffusion pathways in C_{34} and C_{62}

(a) and (e) A1←→A3 for AB100; (b) and (f) A1←→A3 for AB110; (c) and (g) I1←→I2 for AB010; (d) and (h) A1←→I1

A

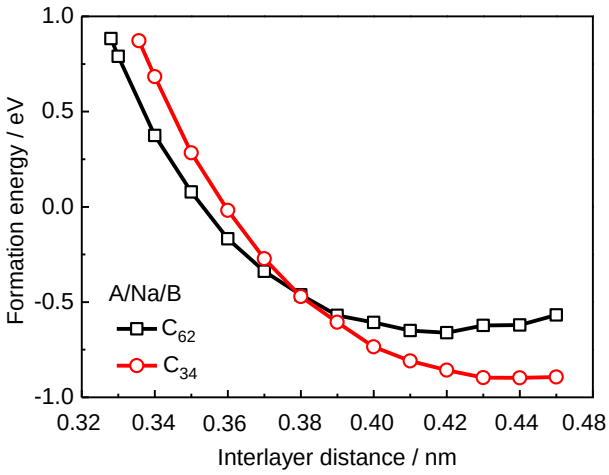

图 S2　C_{62} 和 C_{34} 中 Na 嵌入化合物 A/Na/B 的形成能与层间距的关系

Fig.S2　Formation energy as a function of the average interlayer distances for Na intercalation in the interlayer of C_{62} and C_{34}

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