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Lithium intercalation and diffusion in the TiO2 nanotubes: A first-principles investigation

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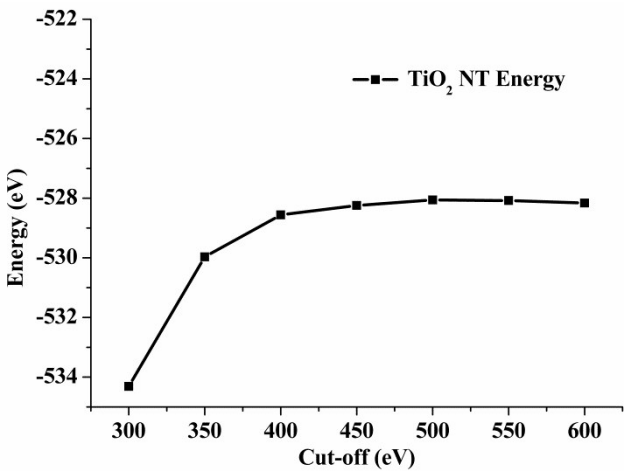
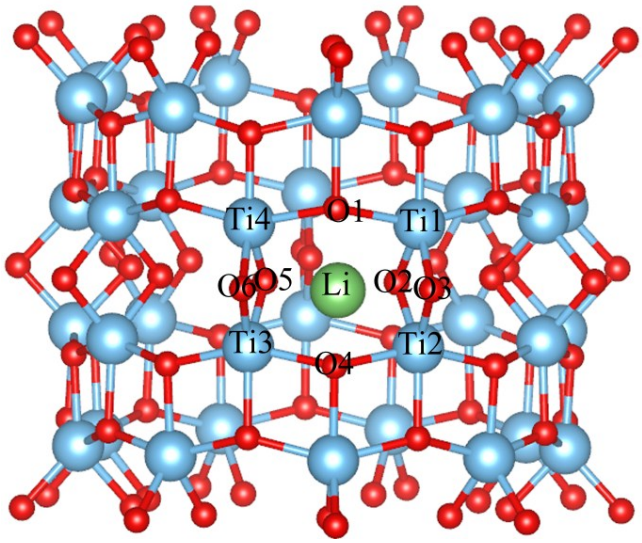
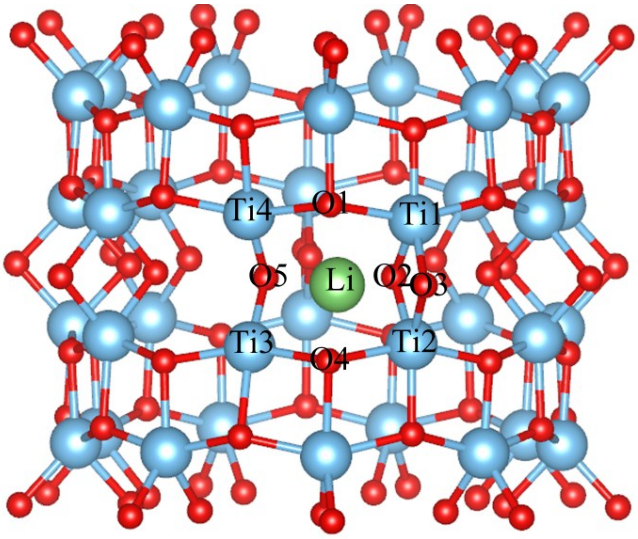


Figure S1. The correspondence of the energy of TiO_2 NT with the cut-off energy.

We performed bader charge analysis to quantitatively calculate the amount of charge transfer between Li and surrounding atoms for perfect and oxygen defective nanotubes. For the transition state listed in Table S1, the net charge of lithium and titanium atoms is obviously decreased while that of surrounding oxygen is increased, when an O_{2c} is removed. It means the transition state of TiO_2 nanotube with oxygen defects is energetically more favorable, therefore the oxygen vacancies lower the energy barrier of lithium diffusion.



(a)



(b)

Figure S2. Li-intercalation sites and the surrounding atoms for perfect and O_{2c}-TiO_2 NTs.

Table S1. Net charge analysis for Li-ion and surrounding atoms along the diffusion pathway (FS: final state, TS: transition state, IS: initial state) in perfect and O_{2c}-TiO_2 NTs.

		Li	Ti1	Ti2	Ti3	Ti4	O1	O2	O3	O4	O5	O6
perfect	FS	0.8819	1.9622	1.9654	1.9685	1.9626	-1.1412	-1.0881	-0.9521	-1.1235	-1.0648	-1.0921
	TS	0.8172	1.9436	1.9405	1.9427	1.9445	-1.2057	-0.9704	-0.9902	-1.207	-0.9918	-0.9728
	IS	0.8813	1.9602	1.9702	1.9702	1.9561	-1.2108	-0.9172	-1.0682	-1.2143	-0.9504	-0.9124
O2c	FS	0.8788	1.9866	1.9864	1.4995	1.502	-1.1568	-1.074	-0.9404	-1.1352	-1.2334	-
	TS	0.7937	1.9391	1.9317	1.5127	1.4946	-1.2099	-0.9918	-0.9691	-1.2196	-1.1245	-
	IS	0.8714	1.9532	1.9488	1.5196	1.5121	-1.2595	-0.9101	-1.0564	-1..2745	-1.0426	-