Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

A Computational Exploration on the 1D TiS_2(en) Nanostructure for Lithium Ion Batteries

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Table S1. Theoretically optimized geometry parameters of the Li_xTiS_2(en) structures with different lithium concentrations in the lowest-energy configurations. The geometry parameters for the experimental XRD measurements are also listed.

Li_xTiS_2(en)	Li configuration	a (Å)	b (Å)	c (Å)	Rüdorff stage
0 (exp) [1]	---	18.44	18.44	9.014	---
0	---	18.58	18.41	9.264	---
0.06	---	18.69	18.75	9.277	---
0.11	(3c, 6a)	18.71	18.79	9.281	---
0.16	(6a, 6b, 6c)	18.81	18.84	9.280	6
0.33	(2a,2b,2c,5a,5b,5c)	18.91	18.91	9.261	3
0.5	(1c,2a,2b,2c,4a,4c,5a,5b,5c)	19.03	19.04	9.260	two-phase (2+3)
0.66	(2a,2b,2c,5a,5b,5c)[a]	19.22	19.22	9.214	2
0.83	(2a,2b,5b)[a]	19.35	19.35	9.171	two-phase (1+2)
1	---	19.61	19.55	8.969	1
1 (exp)[2]	---	19.11	19.11	8.985	1

[a)]The labels of the Li “holes” in the system.

Table S2. Lithium diffusion barriers in selected electrode materials.

Materials	Lithium diffusion barrier (eV)
Si thin film[3]	0.88
h-BAs[4]	0.522
TiS_2[5]	~0.41
SnSe sheet[6]	0.36
PC_6[7]	0.34
Graphite[8]	~0.34
2D YS_2 monolayer[9]	0.33
Graphene[10]	0.327
$NiPS_3$[11]	0.279
TiS_2(en) (this work)	0.27
MoS_2[12]	0.25
VS_2[12]	0.22
CoO_2[13]	0.21
$FePO_4$[13]	0.16
Be_2C monolayer[14]	0.11
Trigonal Mo_2B_2 monolayer[15]	0.023

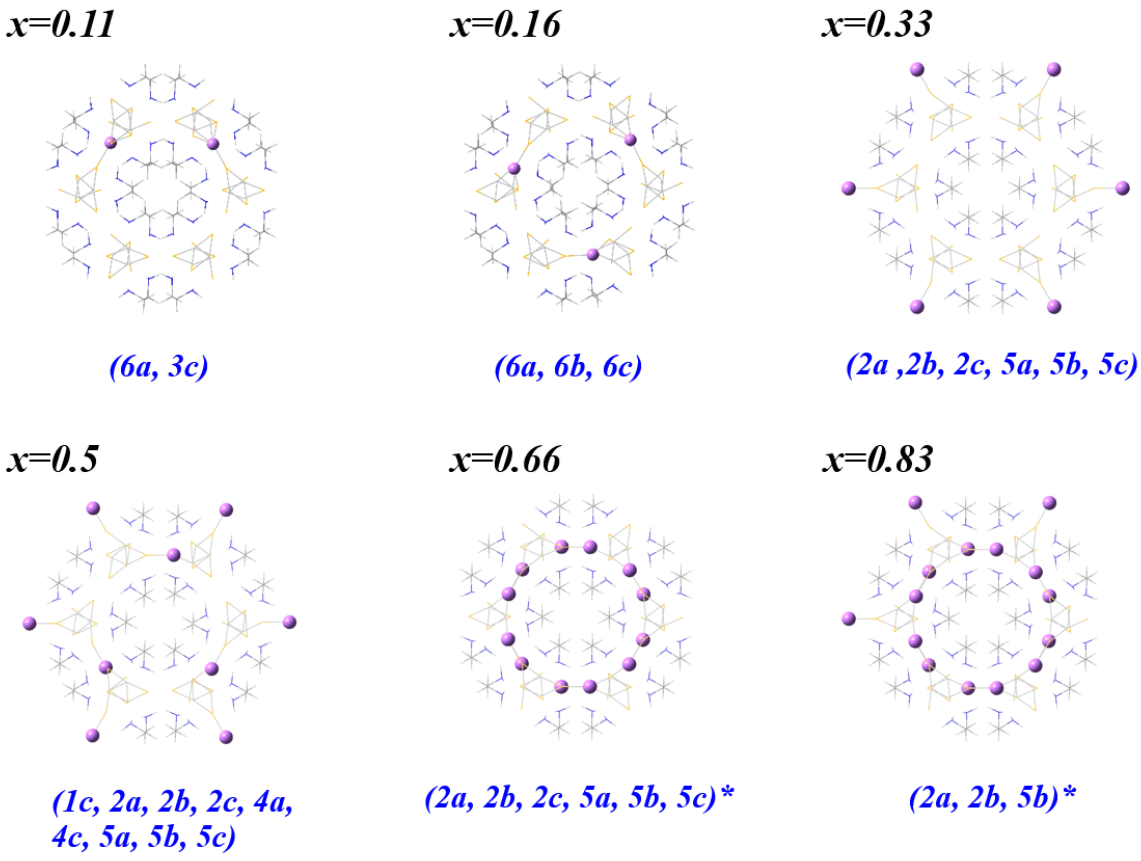

Figure S1. Top view of the lowest-energy configurations under different lithium concentrations. The asterisk marks the configuration of the Li "holes" in the system.

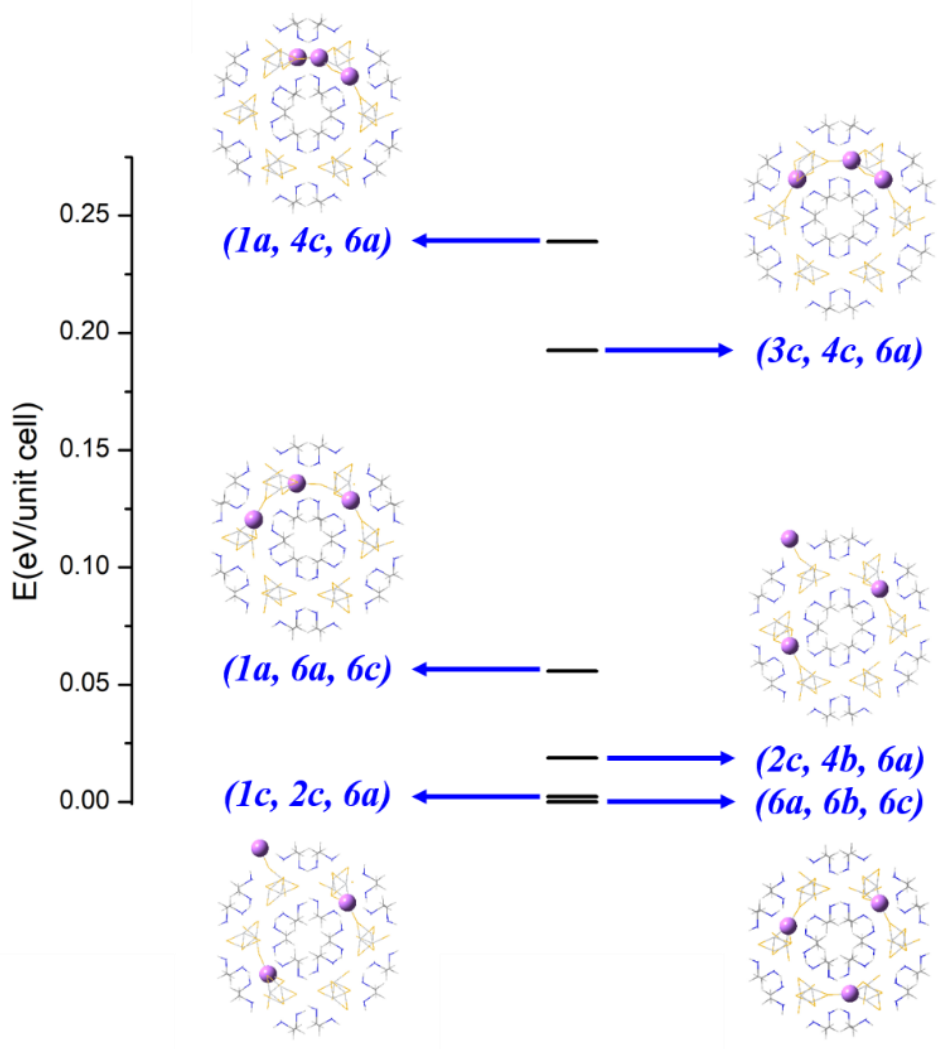

Figure S2. Relative energies of 8 different arrangements in the x=0.16 system.

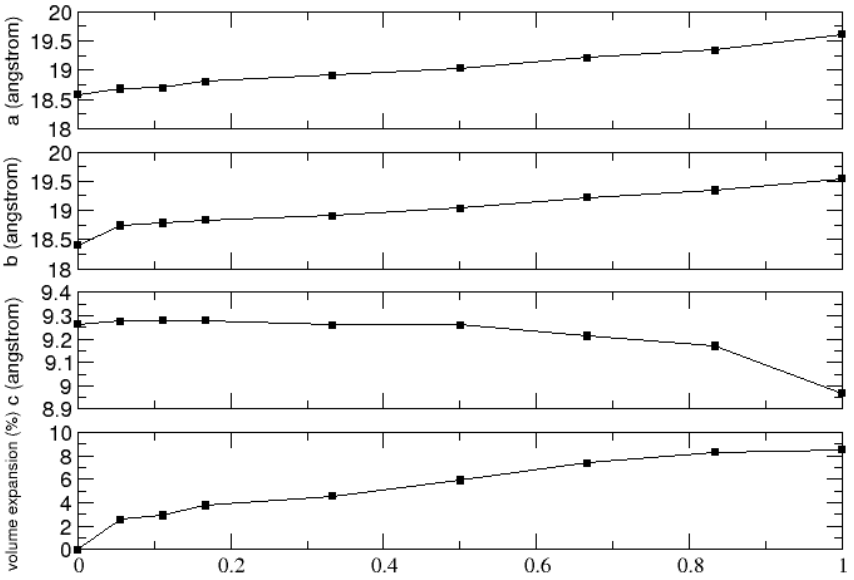

Figure S3. Geometry parameter variation and volume expansion of Li_xTiS_2(en) under different lithium concentrations

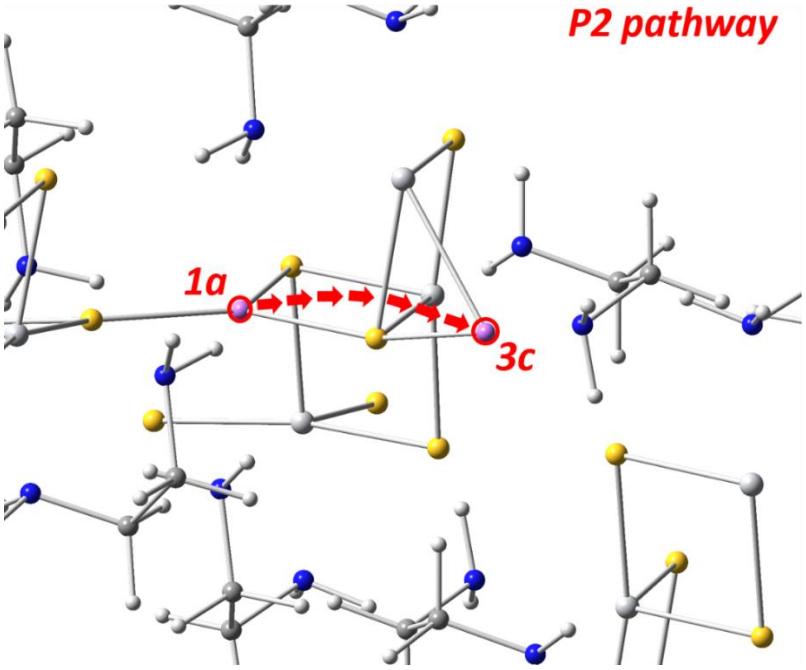

Figure S4. Image of the P2 diffusion pathway of a certain lithium ion in $Li_{0.06}TiS_2$(en).

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