APPENDIX B.

Here we show the ordered structures in 2x2x2 supercells with different arrangement of intercalated Li and O atoms for its corresponding concentrations which were used for simulation of the configurational disorder.

i)   There are five different ordered structures may exist at 25% concentration of the intercalated atoms. A complete optimization of the geometry was performed for each of these structures via minimization of the total energy with respect to the shape and volume of the cell, and the coordinates of all atoms. The symmetry of the cell was not kept fixed within the optimization procedure. The resulting ordered structures with non-metal (O) and metal (Li) intercalated atoms are shown in Figures B1 and B2.
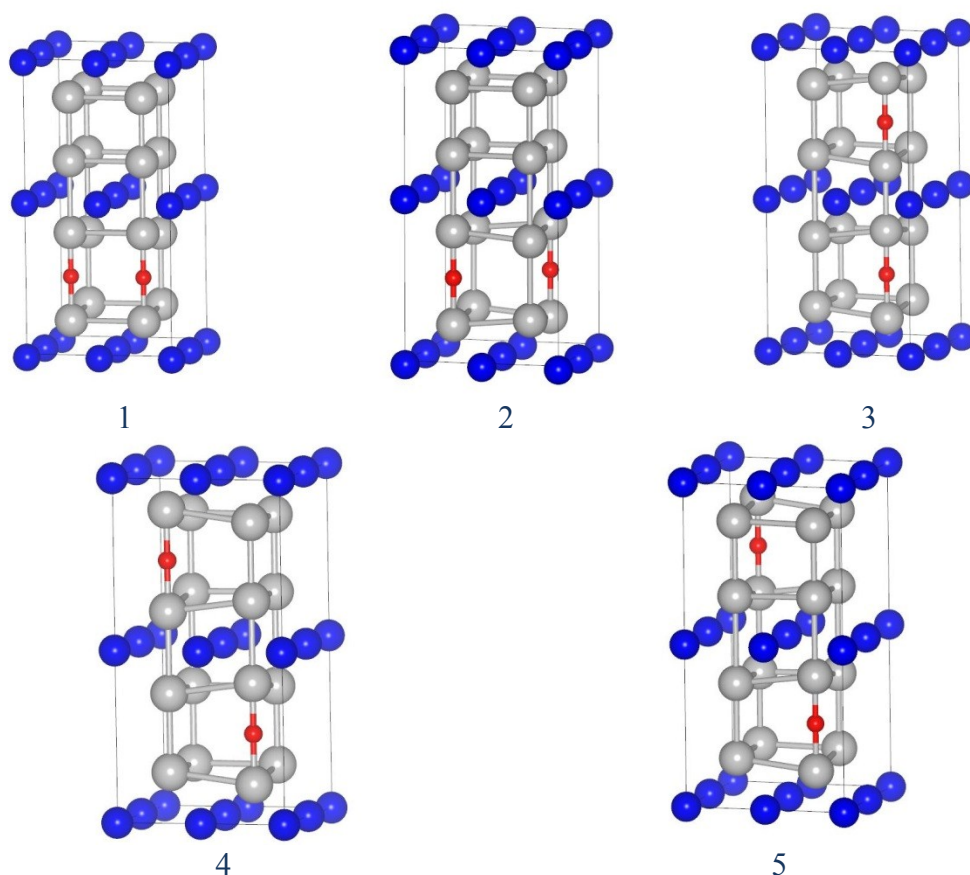

Figure B1. Possible 2x2x2 ordered intercalated structures for the 25% concentration of oxygen atoms. Fe, Si and O atoms are shown by blue, grey and red balls, correspondingly. The numbers denote the ordinal number of structure from Table B1

All characteristics of the used structures are given in Tables B1 – B2. The space symmetry groups of the ordered structures are different: there are orthorhombic Pmmm and Cmmm phases appear along with tetragonal phases. The energies of all ordered structures are within $(<E> \pm 0.4)$ eV / cell.
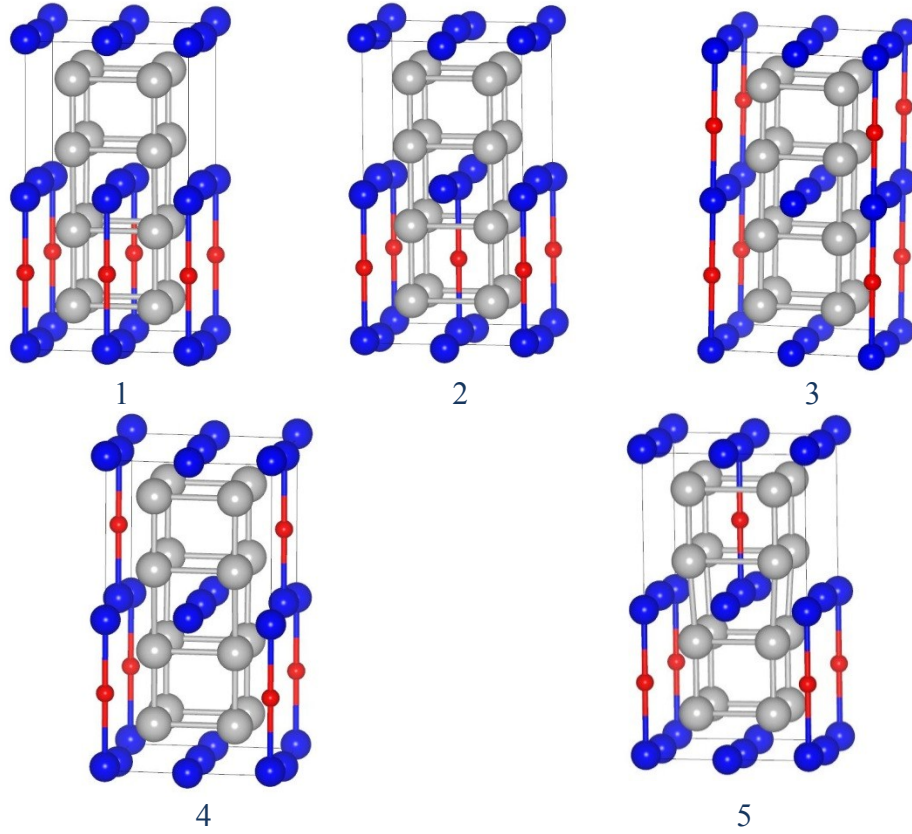
Figure B2. Possible 2x2x2 ordered intercalated structures for the 25% concentration of lithium atoms. Fe, Si and O atoms are shown by blue, grey and red balls, correspondingly. The numbers denote the ordinal number of structure from Table B2

Table B1. The magnetic moments (μ), lattice parameters (a, b and c), total energy (E), total energy per cell, enthalpy of ordered structure formation (H_f(eq.(6)), the weight of each structure (*w*) and the space symmetry group of α-FeSi$_2$ with **25%** concentration of **O** atoms

The number of structure	μ, μ$_B$	a (b) , Å	c , Å	E, eV	E/cell, eV	H_f, eV/N_x	*w*	Space symmetry group
1	0.06	5.42 (5.43)	10.82	-177.264	-22.158	-1.27	8	Pmmm
2	0.10	5.43	10.86	-176.785	-22.098	-1.24	4	P4/mmm
3	0.10	5.42	10.98	-175.442	-21.930	-1.15	4	P4/mmm
4	0.24	5.45(5.44)	10.85	-175.996	-21.999	-1.19	8	Cmmm
5	0.18	5.45	10.87	-175.823	-21.978	-1.18	4	I4/mmm

Table B2. The magnetic moments (μ), lattice parameters (a, b and c), total energy (E), total energy per cell, enthalpy of ordered structure formation ($H_f(eq.(6))$), the weight of each structure (*w*) and the space symmetry group of α-FeSi2 with **25%** concentration of **Li** atoms

The number of structure	μ, μ$_B$	a (b) , Å	c , Å	E, eV	E/cell, eV	H_f, eV/N_x	*w*	Space symmetry group
1	0.42	5.46 (5.65)	10.26	-167.774	-20.972	-0.48	8	Pmmm
2	0.42	5.54	10.39	-167.332	-20.916	-0.45	4	P4/mmm
3	0.26	5.54	10.28	-167.398	-20.925	-0.46	4	P4/mmm
4	0.25	5.62(5.47)	10.28	-167.656	-20.957	-0.47	8	Cmmm

5	0.15	5.54	10.28	-167.755	-20.969	-0.48	4	I4/mmm

ii) For 50% concentration of intercalated atoms there are nine different ordered structures. In each of these structures, a complete optimization of the geometry was carried out. The space symmetry groups of these ordered structures are different; however some structures have the same space group of symmetry. The optimized ordered structures with different space group of symmetry for non-metal (O) and metal (Li) intercalated atoms are shown in Figures B3 and B4. The characteristics of the used structures are given in Tables B3 – B4.

1   2   4
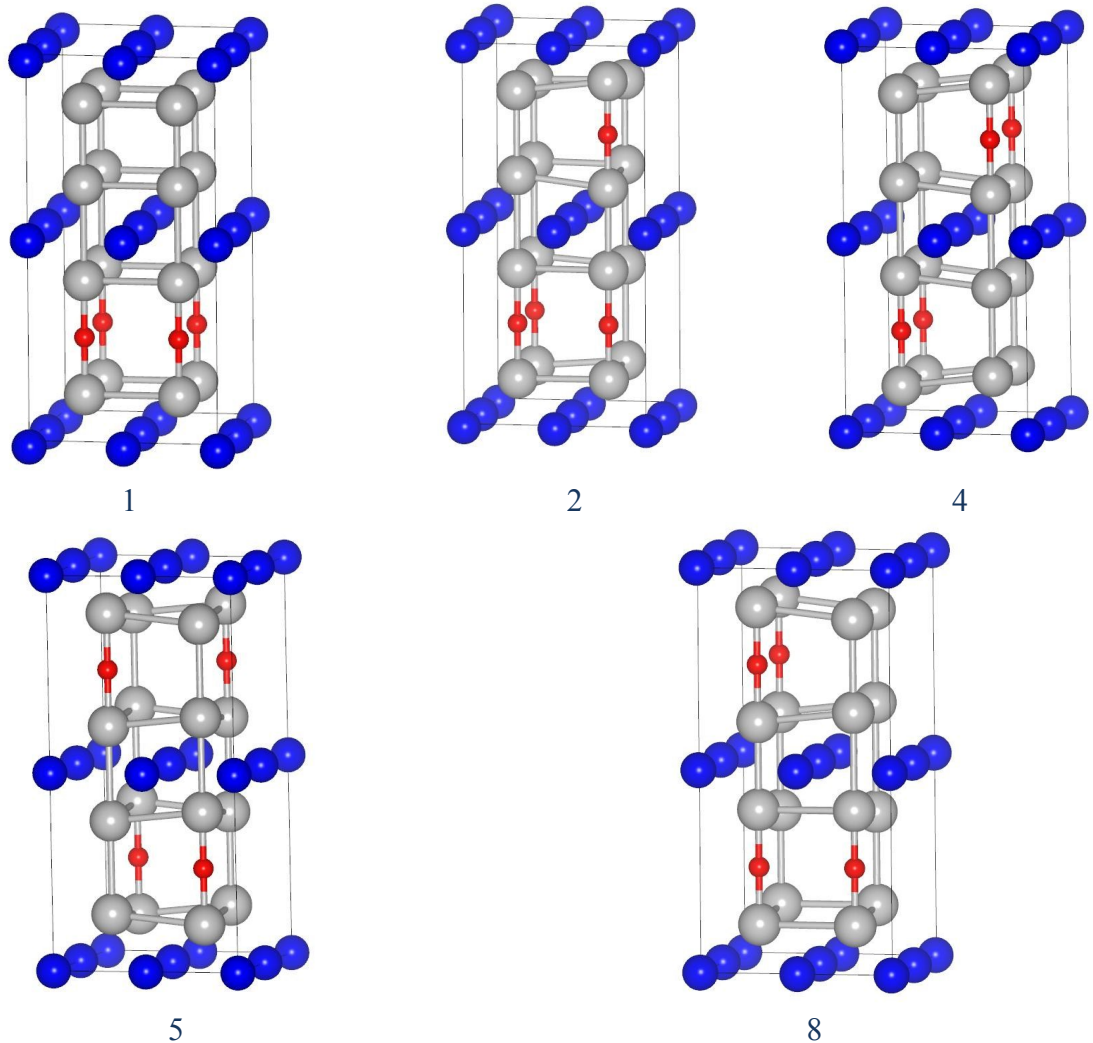

5   8

Figure B3. Possible 2x2x2 ordered intercalated structures for the 50% concentration of oxygen atoms. Fe, Si and O atoms are shown by blue, grey and red balls, correspondingly. The numbers denote the ordinal number of structure from Table B3
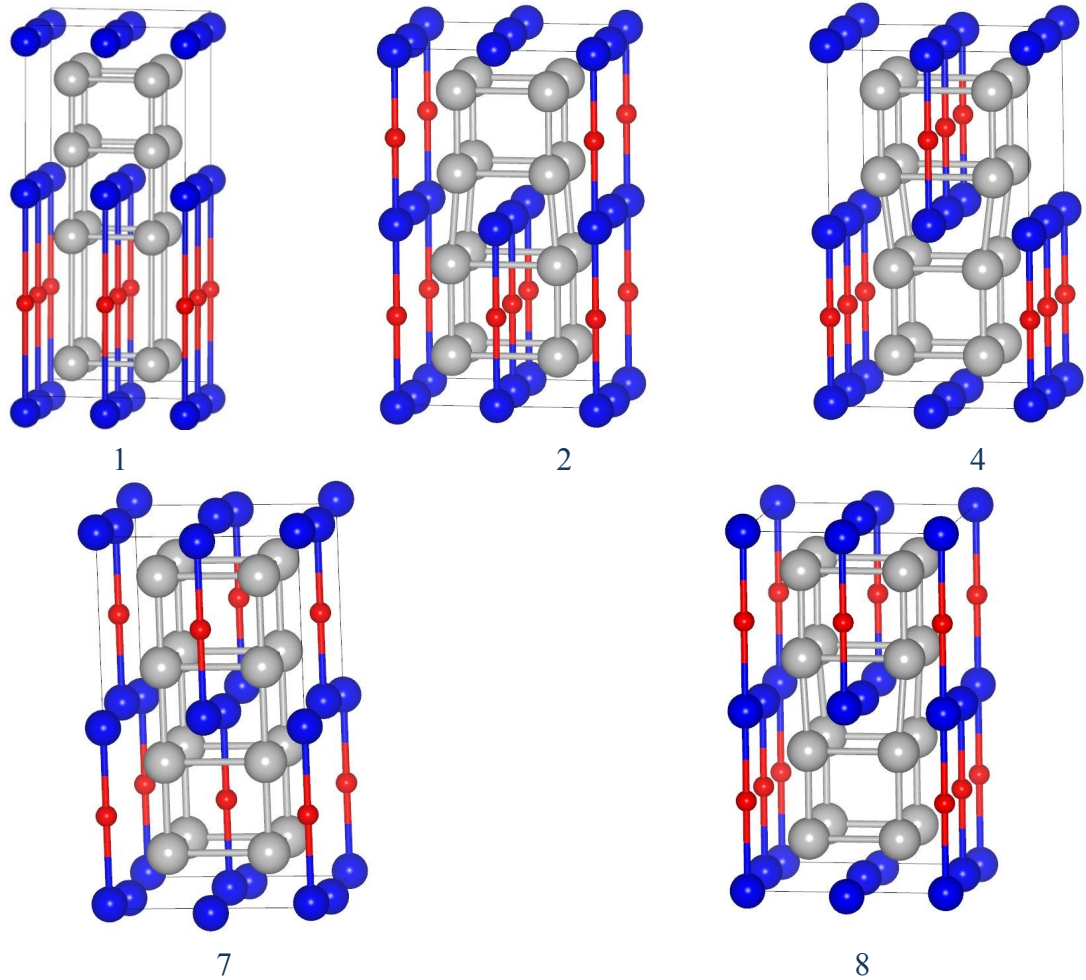
Figure B4. Possible 2x2x2 ordered intercalated structures for the 50% concentration of lithium atoms. Fe, Si and O atoms are shown by blue, grey and red balls, correspondingly. The numbers denote the ordinal number of structure from Table B4

Table B3. The magnetic moments (μ), lattice parameters (a, b and c), total energy (E), total energy per cell, enthalpy of ordered structure formation ($H_f(eq.(6))$), the weight of each structure (w) and the space symmetry group of α-FeSi$_2$ with **50%** concentration of **O** atoms

The number of structure	μ, μ_B	a (b), Å	c, Å	E, eV	E, eV/cell	H_f, eV/ N_x	w	Space symmetry group
1	0.10	5.45	11.10	-194.894	-24.3618	-1.05	2	P4/mmm
2	0.30	5.49 (5.45)	11.31	-192.563	-24.0704	-0.98	24	Pmmm
3	0.35	5.42 (5.53)	11.38	-192.025	-24.0031	-0.96	4	Pmmm
4	0.21	5.46 (5.51)	11.33	-192.444	-24.0555	-0.98	4	Cmmm
5	0.35	5.43 (5.55)	11.33	-191.755	-23.9694	-0.96	8	Pmmm
6	0.35	5.49	11.47	-190.997	-23.8746	-0.93	2	P4/mmm
7	0.32	5.50	11.37	-191.591	-23.9489	-0.95	2	I4/mmm
8	0.27	5.48	11.35	-192.182	-24.0228	-0.97	16	P4$_2$/mmc
9	0.26	5.48	11.27	-192.872	-24.109	-0.99	8	P4/mmm

Table B4. The magnetic moments (μ), lattice parameters (a, b and c), total energy (E), total energy per cell, enthalpy of ordered structure formation ($H_f(eq.(6))$), the weight of each structure (*w*) and the space symmetry group of α-FeSi2 with **50%** concentration of **Li** atoms

The number of structure	μ, μ_B	a (b), Å	c, Å	E/cell, eV	E, eV	$H_{f,\ eV/}$ $\dot{N}_x$	*w*	Space symmetry group
1	0.00	5.36	12.33	-22.069	-176.551	-0.28	2	P4/mmm
2	0.64	5.52 (5.82)	10.36	-21.735	-173.880	-0.20	24	Pmmm
3	0.71	5.75 (5.64)	10.28	-21.667	-173.336	-0.18	4	Pmmm
4	0.66	5.82 (5.52)	10.27	-21.825	-174.598	-0.22	4	Cmmm
5	0.71	5.75 (5.64)	10.31	-21.733	-173.868	-0.20	8	Pmmm
6	0.74	5.71	10.29	-21.649	-173.196	-0.18	2	P4/mmm
7	0.75	5.68	10.41	-21.708	-173.662	-0.19	2	I4/mmm
8	0.72	5.69	10.26	-21.784	-174.272	-0.21	16	P4$_2$/mmc
9	0.75	5.68	10.35	-21.772	-174.177	-0.21	8	P4/mmm