Supplementary material for manuscript "Fe-Si networks and charge/discharge-induced phase transitions in Li_2FeSiO_4 cathode materials"

Space Group Number 33

cell		a	b	c
		11.03838	5.13042	6.26102
Atom	wyckoff	x	y	z
Li	4a	-0.0735	0.7953	-0.0005
Li	4a	0.6595	0.6908	0.2461
Fe	4a	0.6674	0.6980	0.7458
Si	4a	0.4111	0.8081	0.4973
O	4a	0.5860	0.8693	-0.0019
O	4a	0.5500	0.6915	0.4987
O	4a	0.3406	0.7082	0.7171
O	4a	0.3359	0.7098	0.2827

Tab s1. The structural information of the possible Pmnb-cycled phase. The cell is orthonormal, and the atom positions are in direct coordinates

the structural information of Pmnb-cycled phase is shown in Tab.1. Compared with the experimental Pmn21-cycled phase, the proposed Pmnb-cycled phase has the same Fe-Si network but with some cation-centered polyhedra inversed, see fig. s1. The energy of the half-delithiated Pmnb-cycled phase is also slightly lower (0.035eV/f.u.) than the half-delithiated Pmn21-cycled phase. We found that if moving the Li Fe Si atoms (circled out in fig.s1a) across the O atoms to the right direction, the structures in (a) can transform to (b). As the two phases in fig. s1 can be very similar, it is necessary to compared with the experimental results.

The phonon calculation shows that the newly proposed Pmnb-cycled phase is stable, see fig. s2.

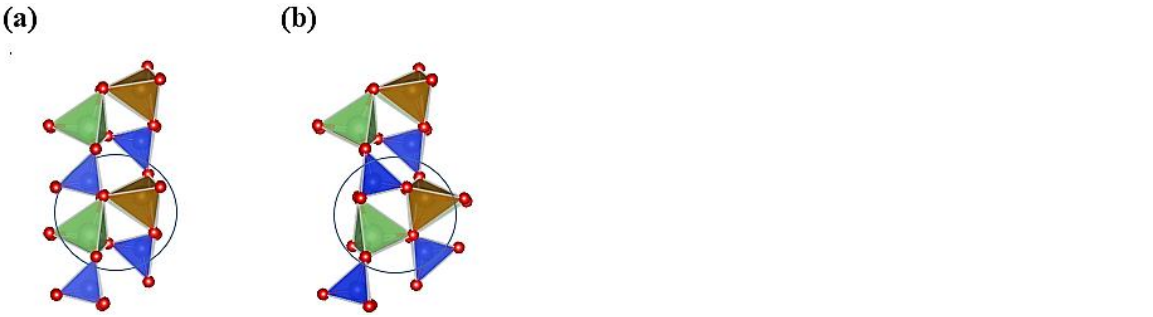

Fig s1. The half-delithiated phase of (a) Pmn21-cycled (b) Pmnb-cycled the difference between the two phases are circled out in the figure.

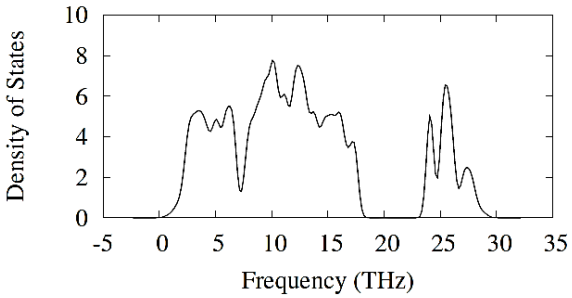

Fig s2. Phonon density of states of the possible Pmnb-cycled phase