Electronic Supplementary Information

Machine Learning Interatomic Potentials in Engineering Perspective for Developing Cathode Materials

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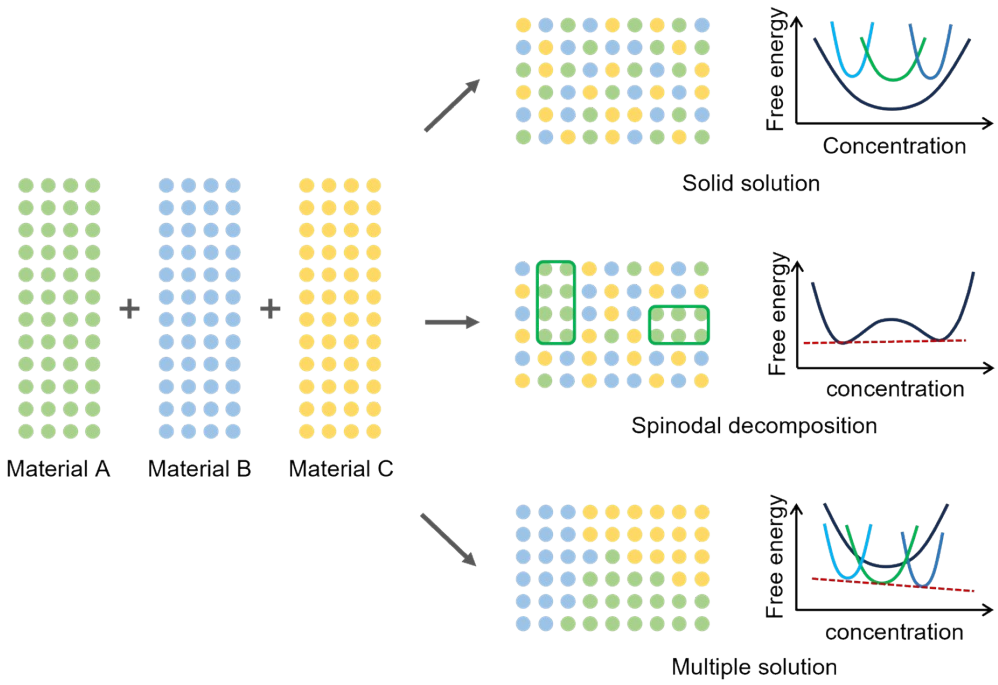

Fig. S1. Possible cases for multi-materials mixing and synthesis reaction.

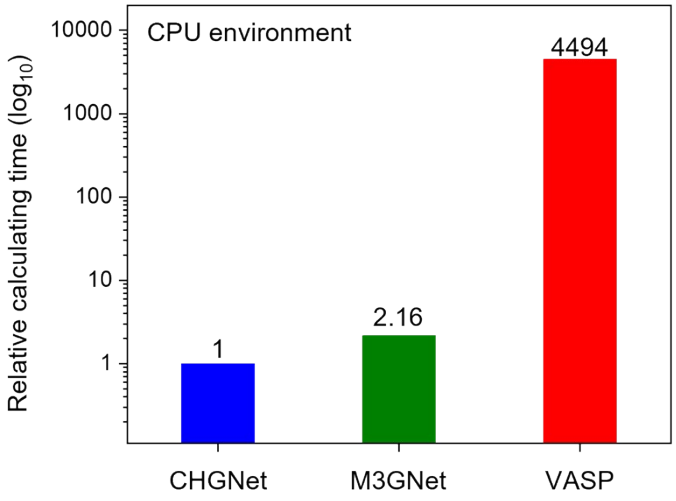

Fig. S2. The overall computational differences between CHGNet, M3GNet, and VASP, with all calculations performed in the same CPU environment. Note that the total computation time may vary depending on the type and performance of the hardware.

Coordinate / ID No.	Ti_1	Ti_2	Ti_3	Ti_4
1	('0.17', '0.50', '0.00')	('0.50', '0.50', '0.00')	('0.83', '0.50', '0.00')	('0.17', '0.00', '0.50')
2	('0.83', '0.00', '0.50')	('0.50', '0.50', '0.00')	('0.83', '0.50', '0.00')	('0.17', '0.00', '0.50')
3	('0.83', '0.00', '0.50')	('0.17', '0.50', '0.00')	('0.83', '0.50', '0.00')	('0.17', '0.00', '0.50')
4	('0.50', '0.00', '0.50')	('0.50', '0.50', '0.00')	('0.83', '0.50', '0.00')	('0.17', '0.00', '0.50')
5	('0.50', '0.00', '0.50')	('0.17', '0.50', '0.00')	('0.50', '0.50', '0.00')	('0.17', '0.00', '0.50')
6	('0.50', '0.00', '0.50')	('0.17', '0.50', '0.00')	('0.50', '0.50', '0.00')	('0.83', '0.50', '0.00')
7	('0.67', '0.50', '0.50')	('0.50', '0.50', '0.00')	('0.83', '0.50', '0.00')	('0.17', '0.00', '0.50')
8	('0.67', '0.50', '0.50')	('0.17', '0.50', '0.00')	('0.83', '0.50', '0.00')	('0.17', '0.00', '0.50')
9	('0.67', '0.50', '0.50')	('0.17', '0.50', '0.00')	('0.50', '0.50', '0.00')	('0.17', '0.00', '0.50')
10	('0.67', '0.50', '0.50')	('0.17', '0.50', '0.00')	('0.50', '0.50', '0.00')	('0.83', '0.50', '0.00')
11	('0.67', '0.50', '0.50')	('0.83', '0.00', '0.50')	('0.83', '0.50', '0.00')	('0.17', '0.00', '0.50')
12	('0.67', '0.50', '0.50')	('0.83', '0.00', '0.50')	('0.50', '0.50', '0.00')	('0.17', '0.00', '0.50')
13	('0.67', '0.50', '0.50')	('0.83', '0.00', '0.50')	('0.50', '0.50', '0.00')	('0.83', '0.50', '0.00')
14	('0.67', '0.50', '0.50')	('0.83', '0.00', '0.50')	('0.17', '0.50', '0.00')	('0.17', '0.00', '0.50')
15	('0.67', '0.50', '0.50')	('0.83', '0.00', '0.50')	('0.17', '0.50', '0.00')	('0.83', '0.50', '0.00')
16	('0.67', '0.50', '0.50')	('0.83', '0.00', '0.50')	('0.17', '0.50', '0.00')	('0.50', '0.50', '0.00')
17	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.83', '0.50', '0.00')	('0.17', '0.00', '0.50')
18	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.50', '0.50', '0.00')	('0.17', '0.00', '0.50')
19	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.50', '0.50', '0.00')	('0.83', '0.50', '0.00')
20	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.17', '0.50', '0.00')	('0.17', '0.00', '0.50')
21	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.17', '0.50', '0.00')	('0.83', '0.50', '0.00')
22	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.17', '0.50', '0.00')	('0.50', '0.50', '0.00')
23	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.83', '0.00', '0.50')	('0.17', '0.00', '0.50')
24	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.83', '0.00', '0.50')	('0.83', '0.50', '0.00')
25	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.83', '0.00', '0.50')	('0.50', '0.50', '0.00')
26	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.83', '0.00', '0.50')	('0.17', '0.50', '0.00')
27	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.83', '0.50', '0.00')	('0.17', '0.00', '0.50')
28	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.50', '0.50', '0.00')	('0.17', '0.00', '0.50')
29	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.50', '0.50', '0.00')	('0.83', '0.50', '0.00')
30	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.17', '0.50', '0.00')	('0.17', '0.00', '0.50')
31	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.17', '0.50', '0.00')	('0.83', '0.50', '0.00')
32	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.83', '0.00', '0.50')	('0.17', '0.00', '0.50')
33	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.17', '0.00', '0.50')
34	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.83', '0.50', '0.00')
35	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.50', '0.50', '0.00')
36	('0.00', '0.50', '0.50')	('0.50', '0.50', '0.00')	('0.83', '0.50', '0.00')	('0.17', '0.00', '0.50')
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39	('0.00', '0.50', '0.50')	('0.17', '0.50', '0.00')	('0.50', '0.50', '0.00')	('0.83', '0.50', '0.00')
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42	('0.00', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.83', '0.50', '0.00')	('0.17', '0.00', '0.50')
43	('0.00', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.50', '0.50', '0.00')	('0.17', '0.00', '0.50')
44	('0.00', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.50', '0.50', '0.00')	('0.83', '0.50', '0.00')
45	('0.00', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.17', '0.50', '0.00')	('0.17', '0.00', '0.50')
46	('0.00', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.17', '0.50', '0.00')	('0.83', '0.50', '0.00')
47	('0.00', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.83', '0.00', '0.50')	('0.17', '0.00', '0.50')
48	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.83', '0.50', '0.00')	('0.17', '0.00', '0.50')
49	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.50', '0.50', '0.00')	('0.17', '0.00', '0.50')
50	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.50', '0.50', '0.00')	('0.83', '0.50', '0.00')
51	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.17', '0.50', '0.00')	('0.17', '0.00', '0.50')
52	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.17', '0.50', '0.00')	('0.83', '0.50', '0.00')
53	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.17', '0.50', '0.00')	('0.50', '0.50', '0.00')
54	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.83', '0.00', '0.50')	('0.17', '0.00', '0.50')
55	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.83', '0.00', '0.50')	('0.83', '0.50', '0.00')
56	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.83', '0.00', '0.50')	('0.50', '0.50', '0.00')
57	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.83', '0.00', '0.50')	('0.17', '0.50', '0.00')
58	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.17', '0.00', '0.50')
59	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.83', '0.50', '0.00')
60	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.50', '0.50', '0.00')
61	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.17', '0.50', '0.00')
62	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.83', '0.00', '0.50')
63	('0.00', '0.50', '0.50')	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.17', '0.00', '0.50')
64	('0.00', '0.50', '0.50')	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.83', '0.50', '0.00')
65	('0.00', '0.50', '0.50')	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.50', '0.50', '0.00')
66	('0.00', '0.50', '0.50')	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')
67	('0.67', '0.00', '0.00')	('0.67', '0.50', '0.50')	('0.83', '0.50', '0.00')	('0.17', '0.00', '0.50')
68	('0.67', '0.00', '0.00')	('0.67', '0.50', '0.50')	('0.50', '0.50', '0.00')	('0.17', '0.00', '0.50')
69	('0.67', '0.00', '0.00')	('0.67', '0.50', '0.50')	('0.50', '0.50', '0.00')	('0.83', '0.50', '0.00')
70	('0.67', '0.00', '0.00')	('0.67', '0.50', '0.50')	('0.17', '0.50', '0.00')	('0.17', '0.00', '0.50')
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72	('0.67', '0.00', '0.00')	('0.67', '0.50', '0.50')	('0.17', '0.50', '0.00')	('0.50', '0.50', '0.00')
73	('0.67', '0.00', '0.00')	('0.67', '0.50', '0.50')	('0.83', '0.00', '0.50')	('0.83', '0.50', '0.00')
74	('0.67', '0.00', '0.00')	('0.67', '0.50', '0.50')	('0.83', '0.00', '0.50')	('0.50', '0.50', '0.00')
75	('0.67', '0.00', '0.00')	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.50', '0.50', '0.00')
76	('0.67', '0.00', '0.00')	('0.33', '0.50', '0.50')	('0.83', '0.50', '0.00')	('0.17', '0.00', '0.50')
77	('0.67', '0.00', '0.00')	('0.33', '0.50', '0.50')	('0.50', '0.50', '0.00')	('0.17', '0.00', '0.50')
78	('0.67', '0.00', '0.00')	('0.33', '0.50', '0.50')	('0.50', '0.50', '0.00')	('0.83', '0.50', '0.00')
79	('0.67', '0.00', '0.00')	('0.33', '0.50', '0.50')	('0.17', '0.50', '0.00')	('0.17', '0.00', '0.50')
80	('0.67', '0.00', '0.00')	('0.33', '0.50', '0.50')	('0.17', '0.50', '0.00')	('0.83', '0.50', '0.00')
81	('0.67', '0.00', '0.00')	('0.33', '0.50', '0.50')	('0.17', '0.50', '0.00')	('0.50', '0.50', '0.00')

82	('0.67', '0.00', '0.00')	('0.33', '0.50', '0.50')	('0.83', '0.00', '0.50')	('0.50', '0.50', '0.00')
83	('0.67', '0.00', '0.00')	('0.33', '0.50', '0.50')	('0.83', '0.00', '0.50')	('0.17', '0.50', '0.00')
84	('0.67', '0.00', '0.00')	('0.33', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.50', '0.50', '0.00')
85	('0.67', '0.00', '0.00')	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.17', '0.00', '0.50')
86	('0.67', '0.00', '0.00')	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.83', '0.50', '0.00')
87	('0.67', '0.00', '0.00')	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.50', '0.50', '0.00')
88	('0.67', '0.00', '0.00')	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.17', '0.50', '0.00')
89	('0.67', '0.00', '0.00')	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.83', '0.00', '0.50')
90	('0.67', '0.00', '0.00')	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')
91	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.83', '0.50', '0.00')	('0.17', '0.00', '0.50')
92	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.50', '0.50', '0.00')	('0.17', '0.00', '0.50')
93	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.50', '0.50', '0.00')	('0.83', '0.50', '0.00')
94	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.17', '0.50', '0.00')	('0.17', '0.00', '0.50')
95	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.17', '0.50', '0.00')	('0.83', '0.50', '0.00')
96	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.17', '0.50', '0.00')	('0.50', '0.50', '0.00')
97	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.83', '0.00', '0.50')	('0.17', '0.00', '0.50')
98	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.83', '0.00', '0.50')	('0.83', '0.50', '0.00')
99	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.83', '0.00', '0.50')	('0.50', '0.50', '0.00')
100	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.83', '0.00', '0.50')	('0.17', '0.50', '0.00')
101	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.17', '0.00', '0.50')
102	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.83', '0.50', '0.00')
103	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.50', '0.50', '0.00')
104	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.17', '0.50', '0.00')
105	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.83', '0.00', '0.50')
106	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.17', '0.00', '0.50')
107	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.83', '0.50', '0.00')
108	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.50', '0.50', '0.00')
109	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.17', '0.50', '0.00')
110	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.83', '0.00', '0.50')
111	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')
112	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.33', '0.50', '0.50')	('0.17', '0.00', '0.50')
113	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.33', '0.50', '0.50')	('0.83', '0.50', '0.00')
114	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.33', '0.50', '0.50')	('0.50', '0.50', '0.00')
115	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.33', '0.50', '0.50')	('0.17', '0.50', '0.00')
116	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.33', '0.50', '0.50')	('0.83', '0.00', '0.50')
117	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.33', '0.50', '0.50')	('0.50', '0.00', '0.50')
118	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')
119	('0.00', '0.00', '0.00')	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.17', '0.00', '0.50')
120	('0.00', '0.00', '0.00')	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.83', '0.50', '0.00')
121	('0.00', '0.00', '0.00')	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.50', '0.50', '0.00')
122	('0.00', '0.00', '0.00')	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')

123	('0.00', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.83', '0.50', '0.00')	('0.17', '0.00', '0.50')
124	('0.00', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.50', '0.50', '0.00')	('0.17', '0.00', '0.50')
125	('0.00', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.50', '0.50', '0.00')	('0.83', '0.50', '0.00')
126	('0.00', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.17', '0.50', '0.00')	('0.17', '0.00', '0.50')
127	('0.00', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.17', '0.50', '0.00')	('0.83', '0.50', '0.00')
128	('0.00', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.50', '0.00', '0.50')	('0.50', '0.50', '0.00')
129	('0.00', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.17', '0.00', '0.50')
130	('0.00', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.83', '0.50', '0.00')
131	('0.00', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.50', '0.50', '0.00')
132	('0.00', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.17', '0.50', '0.00')
133	('0.00', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.83', '0.00', '0.50')
134	('0.00', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')	('0.50', '0.00', '0.50')
135	('0.00', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')
136	('0.00', '0.00', '0.00')	('0.67', '0.00', '0.00')	('0.33', '0.50', '0.50')	('0.67', '0.50', '0.50')
137	('0.00', '0.00', '0.00')	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.67', '0.50', '0.50')
138	('0.00', '0.00', '0.00')	('0.67', '0.00', '0.00')	('0.00', '0.50', '0.50')	('0.33', '0.50', '0.50')
139	('0.33', '0.00', '0.00')	('0.67', '0.00', '0.00')	('0.83', '0.00', '0.50')	('0.83', '0.50', '0.00')

Table S1. The Ti initial coordinates in the rock salt Li2TiA3 (where A represents anions, specifically oxygen and sulfur).

	Li_2TiO_3 (eV / f.u.)						Li_2TiS_3 (eV / f.u.)					
	CHGNet		M3GNet		PBE		CHGNet		M3GNet		PBE	
Rank	Struct. ID	Energy difference	Struct. ID	Energy difference	Struct. ID	Energy difference	Struct. ID	Energy difference	Struct. ID	Energy difference	Struct. ID	Energy difference
1	76	0.00000	83	0.00000	92	0.00000	76	0.00000	92	0.00000	76	0.00000
2	92	0.00008	76	0.00012	83	0.00011	83	0.00029	76	0.00009	104	0.00001
3	83	0.00009	92	0.00025	76	0.00014	92	0.00043	104	0.00013	92	0.00001
4	104	0.00019	104	0.00026	104	0.00025	104	0.00084	83	0.00027	83	0.00008
5	128	0.09589	112	0.12173	122	0.17606	121	0.03024	41	0.01421	81	0.09893
6	46	0.14129	26	0.12176	121	0.17607	122	0.03036	121	0.01424	78	0.09988
7	26	0.14191	46	0.12178	41	0.17628	7	0.03093	46	0.01436	95	0.10034
8	115	0.14211	7	0.12179	46	0.17629	41	0.03094	122	0.01438	56	0.10036
9	121	0.14213	121	0.12181	115	0.17630	115	0.03263	7	0.01442	97	0.10054
10	41	0.14214	115	0.12183	7	0.17630	26	0.03376	115	0.01447	41	0.10308
11	112	0.14215	41	0.12185	26	0.17632	112	0.03401	26	0.01450	7	0.10309
12	7	0.14297	122	0.12189	112	0.17633	46	0.03534	112	0.01453	122	0.10330
13	122	0.14303	70	0.12757	96	0.29016	4	0.07217	70	0.01754	26	0.10332
14	113	0.21568	128	0.12774	101	0.29023	136	0.07396	128	0.01763	121	0.10332
15	117	0.21573	138	0.12991	80	0.29025	2	0.07444	138	0.02137	46	0.10333
16	21	0.21575	2	0.12993	120	0.29057	138	0.07721	136	0.02145	115	0.10333
17	114	0.21578	4	0.12995	61	0.29152	70	0.09876	4	0.02152	112	0.10334
18	116	0.21578	136	0.12996	49	0.29159	96	0.09970	2	0.02176	59	0.11359
19	16	0.21581	64	0.17038	27	0.29183	49	0.10074	116	0.04461	48	0.11501
20	120	0.21582	23	0.17067	12	0.29195	101	0.10170	114	0.04462	54	0.11998
21	17	0.21583	12	0.20911	13	0.29195	80	0.10200	120	0.04477	52	0.12165
22	12	0.21584	36	0.20916	36	0.29205	27	0.10237	12	0.04495	33	0.12174
23	36	0.21585	113	0.20919	116	0.29257	128	0.10289	113	0.04497	29	0.12176
24	119	0.21585	42	0.20923	17	0.29270	61	0.10602	117	0.04502	57	0.13474
25	42	0.21587	21	0.20923	16	0.29291	42	0.10706	17	0.04503	87	0.13963
26	101	0.25222	114	0.20925	19	0.29291	12	0.10724	42	0.04504	17	0.14159
27	27	0.25225	116	0.20925	117	0.29298	17	0.10739	16	0.04510	36	0.14288
28	80	0.25246	120	0.20927	114	0.29353	36	0.10742	119	0.04514	120	0.14350
29	61	0.25248	17	0.20927	113	0.29370	21	0.10761	36	0.04517	119	0.14351
30	49	0.25267	119	0.20929	42	0.29533	116	0.10767	21	0.04521	16	0.14353
31	96	0.25369	117	0.20930	21	0.29586	113	0.10821	44	0.06787	116	0.14359
32	4	0.25459	16	0.20933	119	0.29659	119	0.10915	109	0.06789	117	0.14504
33	136	0.25528	61	0.21345	136	0.34650	117	0.10969	20	0.06791	80	0.16344
34	2	0.25558	49	0.21347	138	0.34653	16	0.11108	14	0.06792	101	0.16347
35	138	0.25583	27	0.21390	2	0.34654	120	0.11309	134	0.06793	49	0.16370

36	70	0.29638	101	0.21394	4	0.34655	114	0.11360	131	0.06794	27	0.16370
37	88	0.41100	80	0.21406	33	0.47284	109	0.13268	9	0.06796	12	0.16408
38	85	0.41104	96	0.21408	50	0.47285	88	0.13309	106	0.06797	42	0.16436
39	20	0.41116	47	0.25043	54	0.47285	43	0.13493	43	0.06798	45	0.16561
40	131	0.41131	63	0.25048	52	0.47292	106	0.13639	88	0.06800	15	0.16597
41	8	0.41182	66	0.25055	20	0.49296	131	0.14148	8	0.06801	18	0.16612
42	43	0.41210	65	0.25066	109	0.49320	134	0.14205	85	0.06803	86	0.16616
43	44	0.41293	109	0.30035	44	0.49326	8	0.14229	80	0.07259	11	0.16617
44	134	0.41333	44	0.30038	9	0.49330	85	0.14254	49	0.07263	89	0.16617
45	109	0.41351	8	0.30043	106	0.49365	20	0.14284	27	0.07268	129	0.16617
46	14	0.41356	9	0.30051	88	0.49368	14	0.14290	96	0.07277	22	0.16618
47	9	0.41410	106	0.30054	85	0.49369	9	0.14460	61	0.07279	21	0.17045
48	106	0.41474	131	0.30064	134	0.49370	44	0.14479	101	0.07280	114	0.17187
49	99	0.44386	134	0.30071	131	0.49370	102	0.14694	67	0.08018	113	0.17364
50	100	0.44403	85	0.30073	43	0.49388	100	0.14719	124	0.08022	108	0.17633
51	91	0.44403	14	0.30079	14	0.49400	91	0.14885	79	0.08026	111	0.17769
52	82	0.44404	43	0.30087	8	0.49401	82	0.14894	68	0.08026	61	0.17863
53	102	0.44406	20	0.30091	77	0.49911	79	0.14930	94	0.08026	96	0.17863
54	77	0.44408	88	0.30092	100	0.50126	77	0.14934	103	0.08036	102	0.18031
55	66	0.44684	118	0.33477	65	0.50921	103	0.14969	1	0.09698	77	0.18038
56	48	0.47577	135	0.33590	64	0.50929	67	0.15033	135	0.09721	99	0.18346
57	97	0.47579	1	0.33592	23	0.50930	68	0.15034	118	0.09723	100	0.18541
58	34	0.47586	6	0.33611	59	0.50982	124	0.15051	6	0.09740	91	0.18542
59	78	0.47586	10	0.34308	99	0.51245	99	0.15056	99	0.10215	82	0.18545
60	57	0.47587	39	0.34318	91	0.51704	94	0.15141	77	0.10221	132	0.19710
61	28	0.47587	58	0.38804	128	0.52099	95	0.18106	102	0.10221	136	0.19862
62	95	0.47587	31	0.41132	70	0.52119	28	0.18330	100	0.10223	2	0.19862
63	59	0.47587	32	0.41151	82	0.52231	48	0.18403	91	0.10224	138	0.19862
64	56	0.47590	53	0.41423	105	0.53542	93	0.18406	82	0.10232	4	0.19864
65	81	0.47590	72	0.42405	48	0.54192	56	0.18476	56	0.11300	67	0.22199
66	105	0.47595	51	0.42408	32	0.54438	59	0.18485	28	0.11303	79	0.22199
67	93	0.47596	30	0.42444	53	0.54439	34	0.18522	97	0.11312	94	0.22199
68	53	0.47803	139	0.42451	31	0.54440	78	0.18541	57	0.11314	103	0.22199
69	6	0.47826	60	0.42513	58	0.54473	81	0.18546	59	0.11315	68	0.22200
70	118	0.47827	71	0.42640	56	0.54648	97	0.18552	95	0.11315	124	0.22200
71	31	0.47829	125	0.42697	57	0.54853	57	0.18553	48	0.11316	14	0.23253
72	135	0.47833	102	0.46092	78	0.54914	53	0.18973	105	0.11319	131	0.23254
73	32	0.47841	100	0.46099	102	0.54991	105	0.19043	93	0.11320	85	0.23254
74	1	0.47887	82	0.46100	34	0.55274	118	0.19073	78	0.11320	88	0.23254

75	58	0.48052	77	0.46101	62	0.55306	58	0.19132	34	0.11321	106	0.23254
76	94	0.48351	91	0.46107	6	0.56025	32	0.19167	81	0.11321	44	0.23254
77	124	0.48362	99	0.46116	1	0.56050	1	0.19183	29	0.11895	134	0.23254
78	79	0.48363	79	0.46977	135	0.56063	6	0.19505	54	0.11901	9	0.23255
79	68	0.48367	103	0.46989	118	0.56089	135	0.19552	33	0.11902	20	0.23256
80	103	0.48375	94	0.46994	93	0.56188	31	0.19628	52	0.11905	43	0.23256
81	67	0.48376	124	0.46997	95	0.56323	15	0.19654	62	0.11906	109	0.23257
82	62	0.50051	68	0.47001	97	0.56328	86	0.19655	50	0.11909	8	0.23260
83	33	0.50053	67	0.47001	81	0.56363	18	0.19662	89	0.13052	93	0.23514
84	52	0.50113	62	0.47598	29	0.56384	129	0.19662	15	0.13057	34	0.24209
85	54	0.50114	33	0.47599	28	0.57064	132	0.19663	111	0.13061	105	0.25253
86	29	0.50114	29	0.47601	103	0.57563	38	0.19668	11	0.13062	28	0.25418
87	50	0.50116	52	0.47618	79	0.57576	89	0.19669	38	0.13063	70	0.28218
88	63	0.56303	50	0.47676	124	0.57644	22	0.19670	129	0.13064	128	0.29447
89	64	0.56456	54	0.47895	68	0.58014	45	0.19684	86	0.13068	62	0.30564
90	10	0.56599	81	0.48660	67	0.58038	108	0.19686	18	0.13070	118	0.30676
91	23	0.56781	28	0.48660	94	0.58412	111	0.19693	22	0.13071	58	0.30751
92	47	0.56849	34	0.48701	47	0.65840	11	0.19698	108	0.13071	135	0.30871
93	65	0.56916	78	0.48736	39	0.65890	52	0.20685	45	0.13072	6	0.30872
94	39	0.57213	95	0.48738	10	0.66083	62	0.20786	132	0.13074	1	0.30873
95	22	0.59553	105	0.48755	63	0.66108	33	0.20800	32	0.13724	53	0.31035
96	132	0.59553	59	0.48757	66	0.66286	50	0.20841	58	0.13729	32	0.31037
97	111	0.59555	57	0.48767	11	0.69813	54	0.21109	31	0.13737	31	0.31572
98	108	0.59563	93	0.48773	108	0.69815	29	0.21145	53	0.13737	47	0.31581
99	89	0.59563	48	0.48781	129	0.69818	23	0.24517	72	0.15194	10	0.31582
100	129	0.59566	97	0.48811	132	0.69820	66	0.24687	125	0.15199	65	0.31587
101	86	0.59570	56	0.48828	22	0.69821	47	0.24711	71	0.15206	66	0.31678
102	18	0.59570	69	0.58886	86	0.69822	39	0.24714	60	0.15403	63	0.32127
103	45	0.59573	127	0.58890	89	0.69823	64	0.24725	30	0.15418	38	0.32163
104	11	0.59574	15	0.59348	15	0.69864	72	0.24771	51	0.15444	64	0.32569
105	38	0.59574	132	0.59357	18	0.69904	63	0.24797	63	0.16854	39	0.32577
106	15	0.59583	3	0.59360	45	0.69910	60	0.24953	65	0.16854	23	0.32727
107	125	0.63088	137	0.59360	38	0.69937	10	0.24964	39	0.16860	60	0.33200
108	139	0.63088	111	0.59362	111	0.69937	65	0.25009	66	0.16860	125	0.33200
109	30	0.63089	5	0.59364	125	0.75367	30	0.25067	64	0.16861	50	0.34271
110	72	0.63096	45	0.59364	51	0.76444	125	0.25070	47	0.16864	30	0.34524
111	71	0.63097	38	0.59370	30	0.76525	5	0.25094	10	0.16868	51	0.34531
112	51	0.63102	18	0.59371	60	0.76603	51	0.25097	23	0.16877	72	0.34532
113	60	0.63138	129	0.59372	139	0.79569	137	0.25111	3	0.17441	71	0.34536

114	137	0.73256	11	0.59372	3	0.79647	71	0.25112	137	0.17616	110	0.36584
115	5	0.73275	89	0.59374	137	0.79702	139	0.25113	139	0.17635	25	0.36711
116	3	0.73304	22	0.59377	5	0.79794	3	0.25114	5	0.17641	40	0.36711
117	24	0.86185	108	0.59377	24	0.88456	19	0.31343	74	0.20175	24	0.36714
118	130	0.86187	86	0.59379	25	0.88464	110	0.31343	69	0.24744	90	0.36721
119	19	0.86189	90	0.88537	110	0.88521	107	0.31348	87	0.27157	37	0.36959
120	37	0.86189	25	0.88538	40	0.88526	25	0.31362	25	0.27164	130	0.37761
121	90	0.86191	24	0.88539	90	0.93657	40	0.31363	19	0.27360	107	0.38049
122	87	0.86192	110	0.88540	107	0.94726	130	0.31368	40	0.27376	13	0.38051
123	107	0.86194	37	0.88540	133	0.98380	24	0.31369	110	0.27396	133	0.38133
124	133	0.86196	13	0.88541	74	1.11262	13	0.31381	130	0.27400	19	0.38136
125	40	0.86197	130	0.88543	98	1.11280	133	0.31384	24	0.27405	5	0.38218
126	110	0.86199	87	0.88544	123	1.11291	37	0.31387	90	0.27410	137	0.38219
127	25	0.86200	19	0.88547	84	1.11299	90	0.31391	13	0.27411	3	0.38220
128	13	0.86202	40	0.88549	127	1.12955	87	0.31412	133	0.27419	74	0.38306
129	84	1.12191	107	0.88555	35	1.18991	73	0.34821	37	0.27428	123	0.38317
130	98	1.12200	133	0.88564	69	1.19625	75	0.36921	107	0.27441	98	0.38319
131	123	1.12201	74	1.16725	55	1.19795	74	0.37972	123	0.34644	139	0.40665
132	74	1.12202	98	1.16736	37	1.30014	84	0.37986	84	0.34691	84	0.41240
133	35	1.16650	84	1.16743	130	1.30524	98	0.38016	98	0.35145	127	0.46686
134	127	1.16663	123	1.16750	72	1.35729	123	0.38033	35	0.38075	69	0.46688
135	55	1.16673	35	1.21006	71	1.35784	55	0.41288	127	0.38132	35	0.46743
136	69	1.16677	55	1.21006	126	1.35852	69	0.41301	55	0.38226	75	0.46773
137	126	1.22921	126	1.31044	75	1.35860	35	0.41313	75	0.42086	55	0.47081
138	75	1.22923	73	1.31049	73	1.35925	127	0.41339	73	0.42094	73	0.47755
139	73	1.22931	75	1.31050	87	1.37097	126	0.47624	126	0.42098	126	0.58851

Table S2. Total energy rankings for each potential of Li_2TiA_3 and structural information for Li-Ti configurations. Energy differences are presented per formula unit. Details on the Structure ID can be found in Table S1.

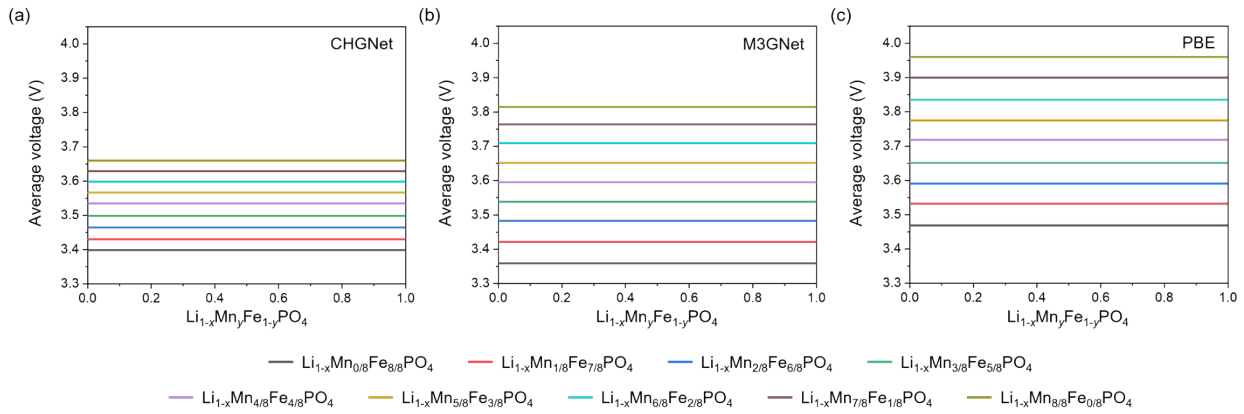

Fig. S3. Calculated average voltages based on the LiMnyFe1-yPO4 and MnyFe1-yPO4 of (a) CHGNet, (b) M3GNet and (c) PBE results.

x = 0.25	CHGNet		M3GNet		PBE		x = 0.75	CHGNet		M3GNet		PBE	
Rank (eV/f.u.)	Struct. ID	Energy difference	Struct. ID	Energy difference	Struct. ID	Energy difference	Rank (eV/f.u.)	Struct. ID	Energy difference	Struct. ID	Energy difference	Struct. ID	Energy difference
1	**3**	0.00000	*2*	0.00000	26	0.00000	1	**24**	0.00000	*25*	0.00000	*2*	0.00000
2	**16**	0.00050	*9*	0.00072	*21*	0.00005	2	**8**	0.00002	*26*	0.00001	***26***	0.00008
3	**17**	0.00070	*6*	0.00159	*6*	0.00242	3	**25**	0.00004	*2*	0.00006	*3*	0.00008
4	**2**	0.00084	*3*	0.00209	28	0.00251	4	**26**	0.00004	*3*	0.00020	***27***	0.00009
5	**13**	0.00236	*21*	0.00357	*3*	0.00343	5	**16**	0.00138	*24*	0.00023	***25***	0.00010
6	**14**	0.00259	*13*	0.00504	**17**	0.00418	6	**27**	0.00196	*27*	0.00031	9	0.00011
7	23	0.00265	14	0.00512	11	0.00943	7	9	0.00205	8	0.00063	***24***	0.00013
8	5	0.00474	17	0.00625	8	0.00944	8	3	0.00212	12	0.00127	**8**	0.00020
9	21	0.00501	16	0.00655	24	0.00944	9	7	0.00335	9	0.00135	15	0.00221
10	20	0.00506	10	0.00669	19	0.00946	10	19	0.00339	7	0.00139	**16**	0.00224
11	4	0.00510	26	0.00712	***2***	0.01242	11	13	0.00340	16	0.00139	19	0.00225
12	27	0.00513	28	0.00879	4	0.01420	12	2	0.00375	20	0.00143	20	0.00225
13	26	0.00517	8	0.01010	20	0.01425	13	6	0.00505	6	0.00146	6	0.00226
14	10	0.00555	11	0.01119	27	0.01425	14	20	0.00514	13	0.00148	7	0.00226
15	22	0.00601	15	0.01142	5	0.01426	15	12	0.00570	19	0.00181	13	0.00228
16	9	0.00612	5	0.01344	*9*	0.01451	16	15	0.00692	15	0.00182	12	0.00239
17	28	0.00664	23	0.01399	22	0.01452	17	18	0.00743	1	0.00242	14	0.01884
18	6	0.00670	4	0.01405	10	0.01453	18	10	0.00751	28	0.00255	28	0.01885
19	11	0.01209	22	0.01481	***13***	0.01454	19	14	0.01027	18	0.00283	23	0.01887
20	24	0.01228	1	0.01619	23	0.01458	20	23	0.01029	21	0.00294	1	0.01887
21	8	0.01336	20	0.01675	**14**	0.01460	21	1	0.01042	23	0.00294	10	0.02534
22	1	0.01573	24	0.01849	**16**	0.01600	22	28	0.01044	14	0.00296	21	0.02534
23	15	0.01582	27	0.01868	18	0.03469	23	21	0.01375	5	0.00304	5	0.02536
24	19	0.01743	19	0.01891	7	0.03470	24	5	0.01927	10	0.00351	18	0.02544
25	18	0.03401	12	0.02074	25	0.03475	25	22	0.03047	22	0.02516	4	0.05920
26	7	0.03406	18	0.02743	1	0.04102	26	17	0.03050	17	0.02518	22	0.05923
27	25	0.03406	7	0.03071	15	0.04108	27	11	0.03833	4	0.02525	17	0.05923
28	12	0.03406	25	0.03094	12	0.06784	28	4	0.04151	11	0.02539	11	0.05930

Table S3. Total energy rank of $Li_{1-x}FePO_4$ (x = 0.25 and x = 0.75) derived from the combination of vacancy contents (x). Structures within the lowest 10% energy range from CHGNet are marked in **bold black** text, and those from M3GNet are marked in *red italic* text. Differences in results due to calculation and boundary conditions in DFT calculations (highlighted orange) are assumed to be less than 0.01 eV per formula unit (f.u.).

x = 0.375	CHGNet		M3GNet		PBE		x = 0.375	CHGNet		M3GNet		PBE	
Rank (eV/f.u.)	Struct. ID	Energy difference	Struct. ID	Energy difference	Struct. ID	Energy difference	Rank (eV/f.u.)	Struct. ID	Energy difference	Struct. ID	Energy difference	Struct. ID	Energy difference
1	**35**	0.00000	*35*	0.00000	20	0.00000	29	43	0.01263	46	0.01706	7	0.01040
2	**56**	0.00011	*24*	0.00293	23	0.00003	30	44	0.01267	4	0.01839	48	0.01042
3	**55**	0.00015	*34*	0.00352	49	0.00004	31	30	0.01273	14	0.01851	***34***	0.01043
4	**34**	0.00065	*12*	0.00372	33	0.00004	32	31	0.01301	28	0.02295	9	0.01043
5	**21**	0.00125	*56*	0.00497	39	0.00004	33	15	0.02634	42	0.02409	*37*	0.01043
6	**19**	0.00154	*21*	0.00515	6	0.00105	34	29	0.02651	29	0.02491	38	0.01043
7	**52**	0.00170	*36*	0.00594	13	0.00106	35	45	0.02860	15	0.02496	*24*	0.01045
8	**36**	0.00176	*25*	0.00642	32	0.00109	36	40	0.02960	32	0.02514	14	0.01045
9	**4**	0.00409	*10*	0.00692	29	0.00161	37	23	0.02977	23	0.02624	*25*	0.01050
10	**50**	0.00444	*37*	0.00698	15	0.00171	38	8	0.02978	5	0.02740	43	0.01260
11	7	0.00523	9	0.00732	**55**	0.00230	39	47	0.03033	47	0.02744	30	0.01265
12	28	0.00523	52	0.00756	**50**	0.00235	40	39	0.03035	27	0.02856	44	0.01269
13	14	0.00532	20	0.00788	***35***	0.00235	41	32	0.03254	22	0.02956	31	0.02204
14	51	0.00624	50	0.00872	***56***	0.00343	42	27	0.03375	33	0.02961	45	0.02557
15	24	0.00636	7	0.01044	1	0.00422	43	6	0.03416	8	0.03055	8	0.02754
16	12	0.00647	19	0.01073	2	0.00430	44	13	0.03417	49	0.03212	47	0.02762
17	2	0.00711	51	0.01101	3	0.00432	45	18	0.03561	13	0.03249	42	0.02764
18	37	0.00722	2	0.01233	*12*	0.00490	46	11	0.03746	40	0.03465	22	0.03886
19	3	0.00745	55	0.01265	**19**	0.00595	47	5	0.03749	39	0.03517	27	0.03986
20	1	0.00788	3	0.01266	***36***	0.00596	48	33	0.03878	45	0.03532	40	0.04693
21	16	0.00877	48	0.01277	**52**	0.00597	49	42	0.03915	6	0.03567	5	0.06351
22	48	0.00941	1	0.01318	***21***	0.00602	50	22	0.03938	11	0.03640	41	0.06353
23	9	0.00943	16	0.01470	51	0.00603	51	49	0.04096	41	0.03855	53	0.06354
24	25	0.01007	31	0.01618	*10*	0.00608	52	41	0.05410	17	0.04003	18	0.06481
25	38	0.01008	38	0.01627	**4**	0.00696	53	53	0.05449	18	0.04050	17	0.06542
26	10	0.01142	30	0.01666	16	0.00801	54	17	0.05552	26	0.04102	26	0.07499
27	20	0.01164	43	0.01667	46	0.00806	55	54	0.05665	54	0.04989	11	0.07556
28	46	0.01239	44	0.01690	28	0.01038	56	26	0.06108	53	0.05637	54	0.11706

Table S4. Total energy rank of $Li_{1-x}FePO_4$ (x = 0.375) derived from the combination of vacancy contents (x). Structures within the lowest 10% energy range from CHGNet are marked in **bold black** text, and those from M3GNet are marked in *red italic* text. Differences in results due to calculation and boundary conditions in DFT calculations (highlighted orange) are assumed to be less than 0.01 eV per formula unit (f.u.).

x = 0.5	CHGNet		M3GNet		PBE		x = 0.5	CHGNet		M3GNet		PBE	
Rank (eV/f.u.)	Struct. ID	Energy difference	Struct. ID	Energy difference	Struct. ID	Energy difference	Rank (eV/f.u.)	Struct. ID	Energy difference	Struct. ID	Energy difference	Struct. ID	Energy difference
1	**15**	0.00000	*24*	0.00000	***56***	0.00000	36	16	0.03944	14	0.02188	38	0.04522
2	**1**	0.00001	*66*	0.00147	*66*	0.00183	37	51	0.03945	39	0.02408	9	0.05411
3	**5**	0.00214	*29*	0.00194	*54*	0.00184	38	23	0.04004	33	0.02414	65	0.06237
4	**8**	0.00285	*8*	0.00293	***36***	0.00188	39	27	0.04059	20	0.02448	32	0.06237
5	**56**	0.00342	*5*	0.00315	**15**	0.00208	40	14	0.04078	19	0.02470	53	0.06238
6	**47**	0.00629	*42*	0.00318	*17*	0.00290	41	20	0.04081	65	0.02477	18	0.06238
7	**42**	0.00635	*70*	0.00358	***63***	0.00293	42	44	0.04112	26	0.02519	33	0.06238
8	**70**	0.00779	*56*	0.00372	*70*	0.00390	43	65	0.04115	18	0.02542	19	0.06240
9	**66**	0.00919	*54*	0.00399	***5***	0.00437	44	59	0.04171	46	0.02554	68	0.06244
10	**35**	0.01123	*1*	0.00485	***8***	0.00442	45	39	0.04176	58	0.02560	39	0.06244
11	**36**	0.01309	*36*	0.00566	***35***	0.00955	46	46	0.04229	31	0.02576	69	0.06253
12	**24**	0.01352	*47*	0.00791	*47*	0.01014	47	52	0.04246	57	0.02611	20	0.06433
13	**63**	0.01396	*17*	0.00821	***42***	0.01024	48	68	0.04310	38	0.02636	51	0.06434
14	**17**	0.01427	*63*	0.00914	***1***	0.01281	49	53	0.04324	59	0.02636	25	0.06435
15	54	0.01430	35	0.00915	*29*	0.01618	50	45	0.04371	60	0.02646	31	0.06435
16	29	0.01809	15	0.01009	60	0.01633	51	69	0.04404	51	0.02695	46	0.06438
17	60	0.02357	37	0.01611	***24***	0.01943	52	30	0.04520	6	0.02722	11	0.06439
18	31	0.02372	34	0.01614	58	0.02002	53	6	0.04603	55	0.02737	57	0.06441
19	4	0.02912	67	0.01624	62	0.02347	54	33	0.04693	48	0.02768	59	0.06441
20	62	0.03183	25	0.01664	34	0.02349	55	58	0.04830	49	0.02882	13	0.06442
21	34	0.03185	16	0.01678	16	0.02350	56	3	0.05020	68	0.02895	12	0.06442
22	67	0.03263	44	0.01758	4	0.02560	57	7	0.05030	53	0.02934	26	0.06445
23	9	0.03265	22	0.01770	48	0.03086	58	32	0.05041	13	0.03012	28	0.06487
24	19	0.03398	27	0.01787	41	0.03091	59	2	0.05102	7	0.03181	6	0.06492
25	18	0.03403	23	0.01794	44	0.03096	60	57	0.05135	52	0.03276	43	0.06496
26	64	0.03436	32	0.01837	55	0.03145	61	26	0.05148	45	0.03292	21	0.06498
27	13	0.03480	64	0.01882	67	0.03150	62	38	0.05292	21	0.03439	40	0.07161
28	12	0.03488	30	0.01899	37	0.03166	63	40	0.05305	50	0.03449	45	0.07162
29	11	0.03489	4	0.01942	30	0.03837	64	25	0.05350	28	0.03486	14	0.07166
30	55	0.03592	40	0.01987	27	0.03842	65	28	0.05960	43	0.03545	2	0.07264
31	22	0.03608	69	0.01991	49	0.03842	66	21	0.06225	12	0.03603	3	0.07266
32	41	0.03622	9	0.02045	23	0.03843	67	43	0.06624	3	0.04177	7	0.07267
33	48	0.03709	11	0.02111	22	0.03845	68	50	0.06630	2	0.04191	50	0.08640
34	37	0.03711	41	0.02146	52	0.04330	69	61	0.07831	61	0.04280	61	0.14306
35	49	0.03712	62	0.02183	64	0.04521	70	10	0.09159	10	0.06442	10	0.14310

Table S5. Total energy rank of $Li_{1-x}FePO_4$ (0.5) derived from the combination of vacancy contents (x). Structures within the lowest 10% energy range from CHGNet are marked in **bold black** text, and those from M3GNet are marked in *red italic* text. Differences in results due to calculation

and boundary conditions in DFT calculations (highlighted orange) are assumed to be less than 0.01 eV per formula unit (f.u.).

x = 0.625	CHGNet		M3GNet		PBE		x = 0.625	CHGNet		M3GNet		PBE	
Rank (eV/f.u.)	Struct. ID	Energy difference	Struct. ID	Energy difference	Struct. ID	Energy difference	Rank (eV/f.u.)	Struct. ID	Energy difference	Struct. ID	Energy difference	Struct. ID	Energy difference
1	**47**	0.00000	*22*	0.00000	*22*	0.00000	29	56	0.01314	53	0.00787	*56*	0.02052
2	**53**	0.00369	*56*	0.00010	**1**	0.00000	30	45	0.01465	20	0.00921	*29*	0.02341
3	**55**	0.00433	*54*	0.00019	7	0.00002	31	37	0.01736	11	0.00936	*32*	0.02343
4	**21**	0.00443	*32*	0.00104	2	0.00005	32	23	0.01816	36	0.01098	33	0.02714
5	**54**	0.00464	*45*	0.00105	*6*	0.00519	33	42	0.02826	49	0.01434	35	0.04554
6	**13**	0.00530	*47*	0.00128	5	0.00521	34	25	0.02829	12	0.01500	30	0.04563
7	**32**	0.00543	*6*	0.00128	*47*	0.00521	35	15	0.02964	30	0.01500	42	0.04563
8	**1**	0.00555	*50*	0.00169	**21**	0.00522	36	4	0.03119	10	0.01531	34	0.04564
9	**22**	0.00592	*27*	0.00183	26	0.00996	37	16	0.03131	25	0.01537	10	0.04858
10	**41**	0.00633	*29*	0.00188	43	0.00996	38	28	0.03328	17	0.01542	18	0.04858
11	5	0.00646	43	0.00205	*45*	0.00997	39	44	0.03431	44	0.01722	8	0.04859
12	26	0.00715	14	0.00209	20	0.00998	40	35	0.03509	8	0.01760	15	0.04861
13	7	0.00727	23	0.00210	*50*	0.00998	41	18	0.03601	35	0.02018	44	0.04862
14	6	0.00871	48	0.00211	**13**	0.00999	42	30	0.03601	15	0.02020	17	0.04863
15	27	0.00909	13	0.00232	11	0.00999	43	8	0.03717	34	0.02050	25	0.04863
16	9	0.00919	33	0.00234	*27*	0.00999	44	10	0.03724	42	0.02065	49	0.04864
17	29	0.00921	38	0.00238	19	0.01000	45	12	0.03852	28	0.02119	24	0.05904
18	2	0.00927	37	0.00241	9	0.01003	46	49	0.03957	39	0.02378	12	0.05904
19	11	0.00934	5	0.00255	14	0.01004	47	24	0.03958	31	0.02386	28	0.05904
20	33	0.00937	21	0.00261	48	0.01005	48	34	0.04142	4	0.02404	51	0.05978
21	50	0.00937	26	0.00304	23	0.01005	49	17	0.04182	52	0.02412	16	0.09468
22	36	0.00939	9	0.00542	**53**	0.01389	50	51	0.04186	24	0.02634	4	0.09535
23	48	0.00941	19	0.00565	**55**	0.01390	51	3	0.04528	18	0.02648	39	0.09985
24	38	0.01090	41	0.00579	*54*	0.01396	52	40	0.04791	51	0.02998	3	0.09985
25	43	0.01121	7	0.00742	37	0.01936	53	39	0.04797	40	0.03354	40	0.10001
26	19	0.01178	55	0.00756	36	0.01936	54	46	0.05226	3	0.03449	52	0.10005
27	14	0.01181	2	0.00758	38	0.01938	55	31	0.06258	46	0.03515	31	0.10199
28	20	0.01313	1	0.00759	**41**	0.01940	56	52	0.06360	16	0.03556	46	0.10589

Table S6. Total energy rank of $Li_{1-x}FePO_4$ (x = 0.625) derived from the combination of vacancy contents (x). Structures within the lowest 10% energy range from CHGNet are marked in **bold black** text, and those from M3GNet are marked in *red italic* text. Differences in results due to calculation and boundary conditions in DFT calculations (highlighted orange) are assumed to be less than 0.01 eV per formula unit (f.u.).

Through the manuscript, we discovered that MLIPs are unable to accurately predict phase formation and voltage profiles during the charging process. Given that voltage inference is a

critical factor in electrode material development, *ab initio* calculations are essential. However, as shown in Figure S1, DFT calculations require significantly more time compared to MLIPs. It is inefficient to determine all possible configurations of Li ion vacancies using DFT calculation alone. If MLIPs can effectively infer Li ion configurations, they would be valuable as a preprocessing step before DFT calculations. Based on this assumption, Table Sx1-Sx4 illustrates how well the most stable energy structures predicted by MLIPs align with PBE calculation results. Although there is a need for cross-validation through multiple materials due to the limited comparison data in this study, MLIPs appear to be effective in inferring the arrangement of Li ions during the delithiation process.

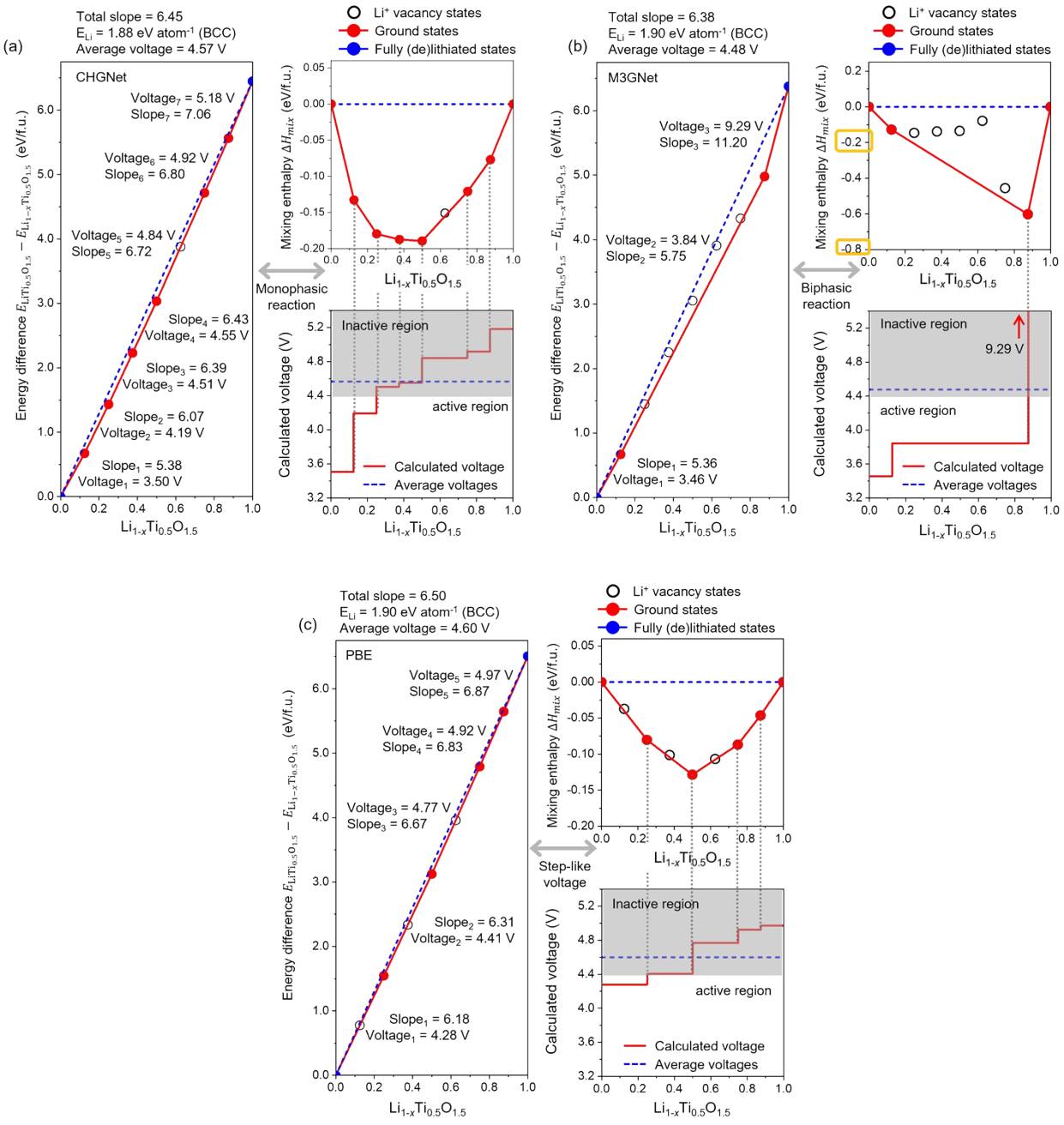

Fig. S4. Energy difference between fully lithiated and delithiated state of $Li_{1-x}Ti_{0.5}O_{1.5}$ (left). Formation energy of mixing enthalpy (top right). Calculated voltage based on formation energy of mixing enthalpy (bottom right). (a) CHGNet, (b) M3GNet and (c) PBE.

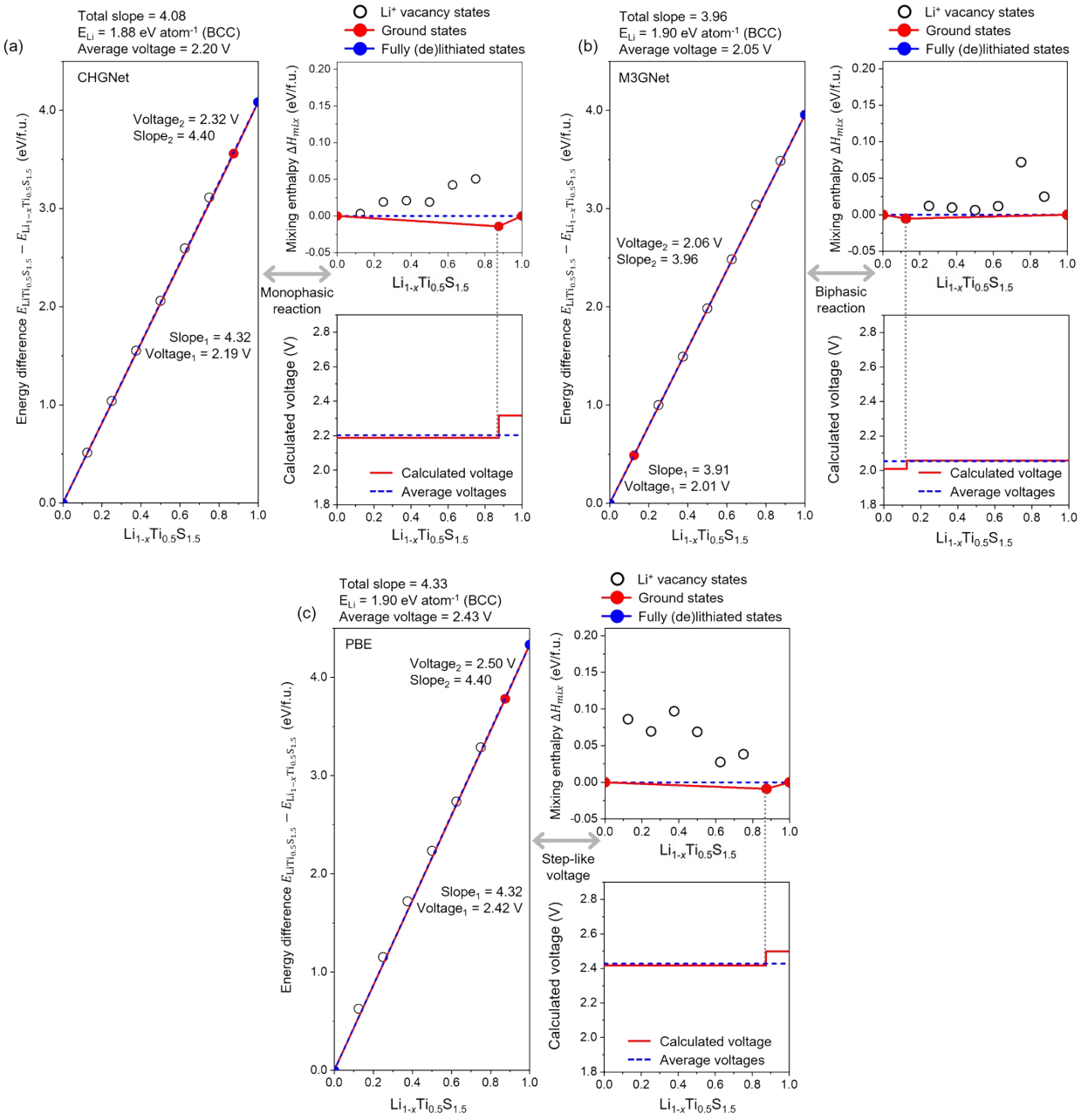

Fig. S5. Energy difference between fully lithiated and delithiated state of $Li_{1-x}Ti_{0.5}S_{1.5}$ (left). Formation energy of mixing enthalpy (top right). Calculated voltage based on formation energy of mixing enthalpy (bottom right). (a) CHGNet, (b) M3GNet and (c) PBE.

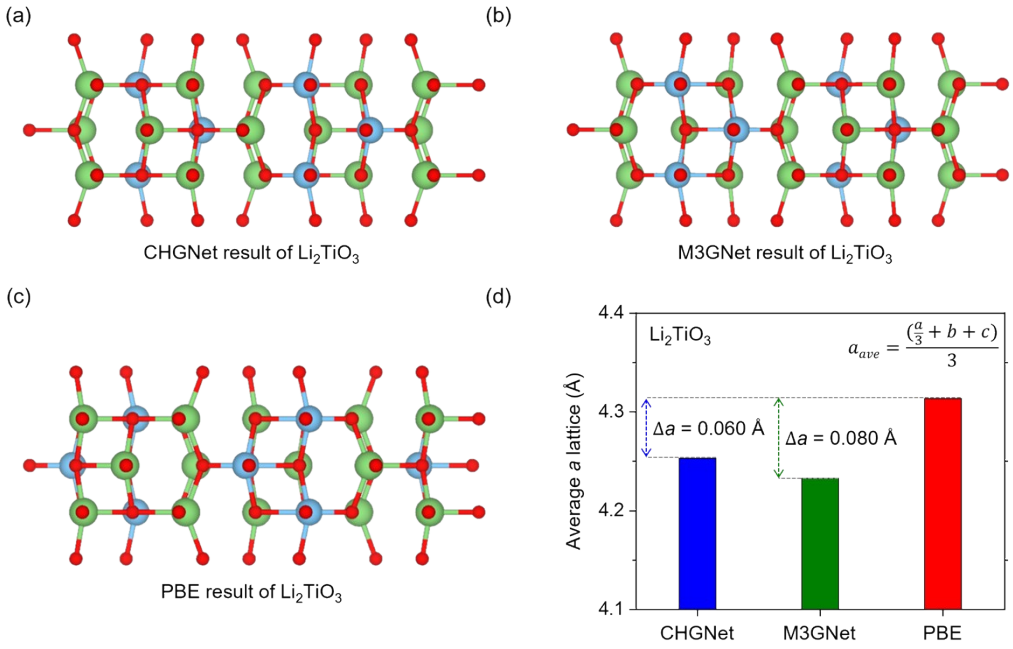

Fig S6. (a-c) Schematic diagrams and atomic configuration of Li_2TiO_3 with the lowest energy values calculated. (d) Lattice parameters as determined by CHGNet, M3GNet, and PBE results.

Spinel $LiMnO_2$			
(Å)	CHGNet	M3GNet	PBE
a lattice	2.874	2.878	2.869
b lattice	4.634	4.680	4.647
c lattice	5.820	5.816	5.837
Shortest Mn–O	1.943	1.938	1.942
Longest Mn–O	2.334	2.349	2.34
Average Mn–O	2.084	2.091	2.087

Table S7. Comparison of lattice parameters and Mn–O of MnO_6 octahedral about $LiMnO_2$ spinel structure.

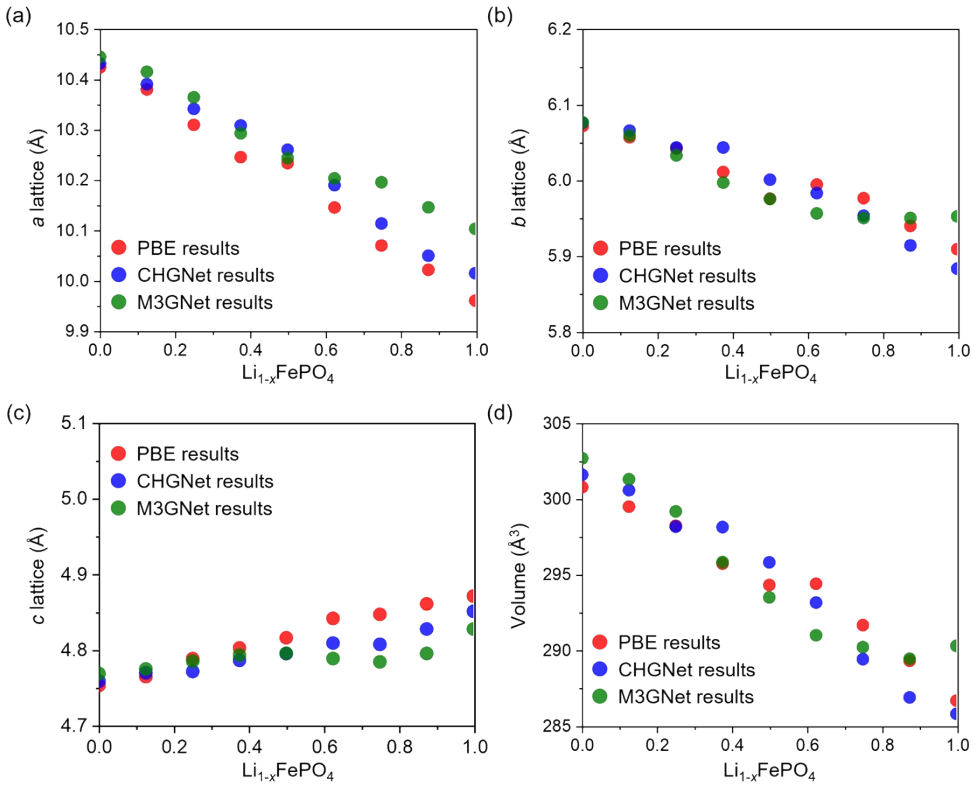

Fig S7. Displacements in lattice constants and volume of $Li_{1-x}FePO_4$ as a function of Li ion vacancy content of (x), using PBE and MLIPs.

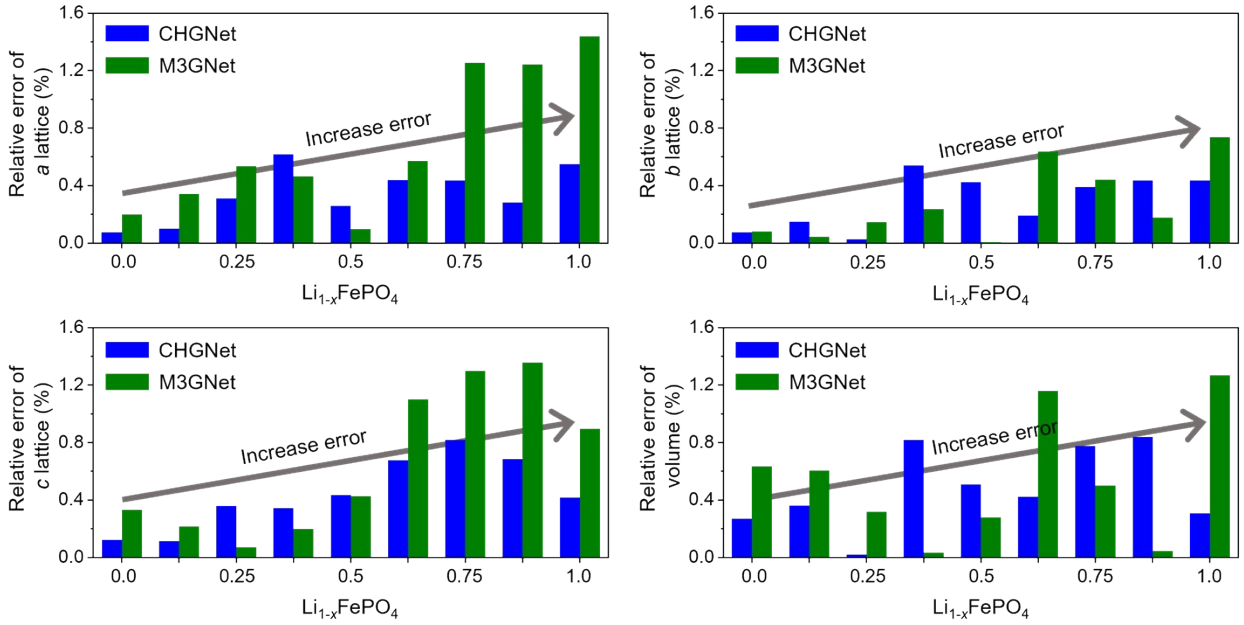

Fig S8. Changes in relative errors of lattice parameters and volume during the delithiation process in $Li_{1-x}FePO_4$. The results from PBE and MLIPs were compared, showing a tendency of increasing relative errors as the amount of Li ion vacancy (x) increases.