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Energy Materials

Supplementary Material: Toward Unraveling the Mechanism of Doping in the Lithium Iron Phosphate

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Contents

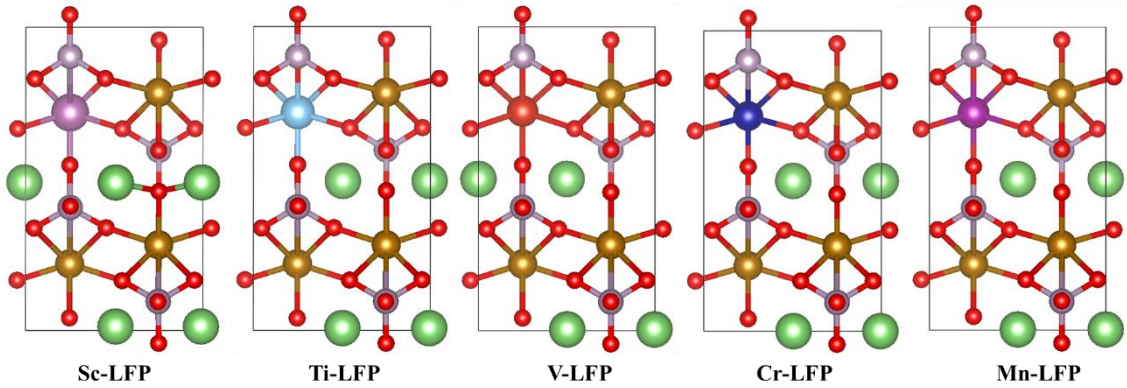
1. Basic research contents and calculation methods

All the calculations of the TM-models considered in this work were conducted by using density functional theory (DFT) on the basis of projector augmented wave (PAW) and Vienna Ab-initio Simulation Package (VASP) [1, 2]. Detailly, the general gradient approximation (GGA) method with the parameters of Perdew-Burke-Ernzerhof (PBE) was used for the exchange-correlation funcitonal in this work [3]. The cutoff energy for the lattice optimization and properties-related calculations were set as 500 eV for the expansion of plane-waves. In order to consider the possible magnetization in the doping model, spin-polarized DFT method was used in the calculation process. The temperature width was set as 0.1 eV by using the Gaussian electronic smearing method for the energy minimization of the electronic steps [4].

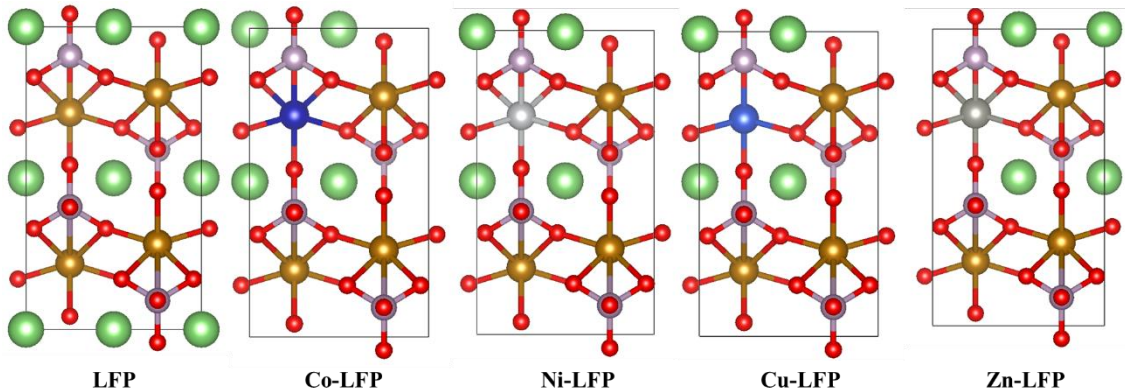
Supplementary Table 1. Six screening criteria used to screen the electrochemical properties of TM-LFP.

Screening criteria	Properties (importance)	Description
Changes of cell volume	Stability (premise)	The relative stability of lattice structure and cell volume are the premise for the excellent electrochemical properties of the corresponding structures. **Directions:** (1) smaller lattice parameters changes; (2) smaller cell volume changes.
Band gaps	Electronic conductivity (key)	Small band gaps are a necessary prerequisite for the electrode material to have good electronic conduction capability. **Directions:** smaller band gaps refer to higher electronic conductivity.
Doping formation energy	Formation (key)	Lower formation energy is the determining factor that doping models can successfully synthesize experimentally. **Directions:** the more negative formation energy refers to material easier to be formed.
Elasticity	Stability (premise)	Good elasticity is an important parameter for electrode materials to be able to restore their original appearance as much as possible after multiple charge-discharge cycles. **Directions:** including linear compressibility and shear strength.
Anisotropy	Stability (premise)	High anisotropy makes the electrode material prone to cracks and reduces its cycle performance. **Directions:** higher isotropy, fewer cracks.
Operating voltage	For higher energy density (key)	The high operating voltage of the electrode material allows the battery made with it to have a high energy density. **Directions:** higher voltage, higher energy density.

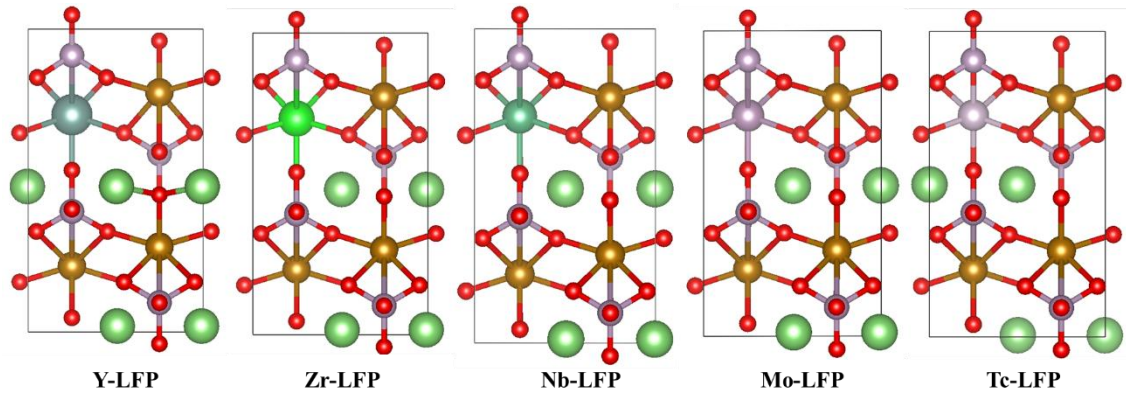
2. Screening for lower lattice cell volume changes



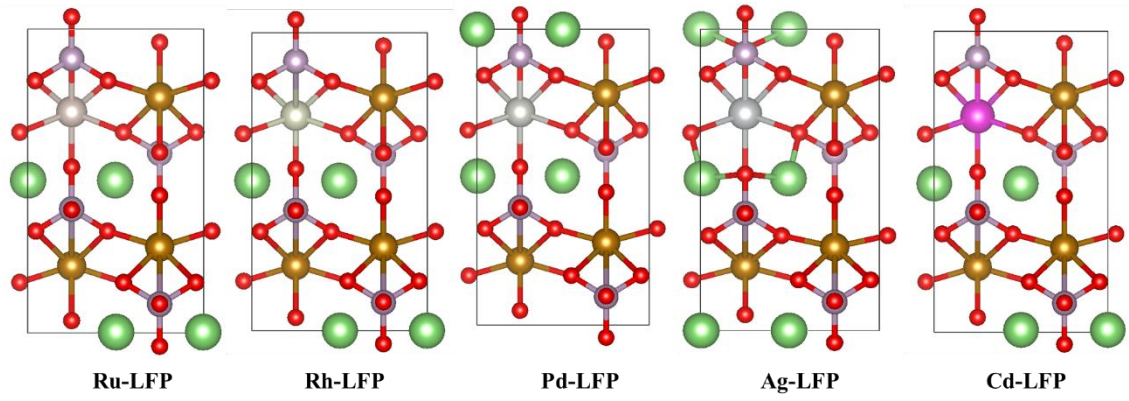
Supplementary Figure 1. Optimized lattice of TM (TM = Sc, Ti, V, Cr and Mn) doped LFP.



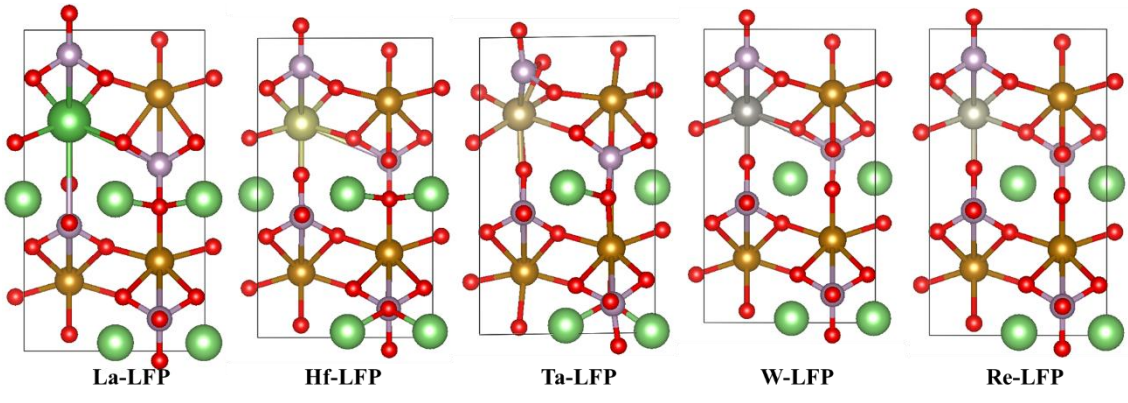
Supplementary Figure 2. Optimized lattice of TM (TM = Fe, Co, Ni, Cu and Zn) doped LFP.



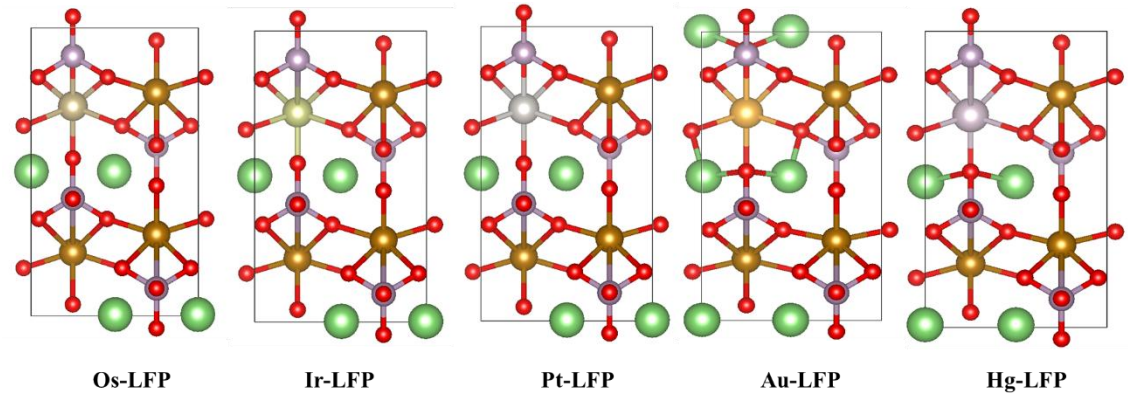
Supplementary Figure 3. Optimized lattice of TM (TM = Y, Zr, Nb, Mo and Tc) doped LFP.



Supplementary Figure 4. Optimized lattice of TM (TM = Ru, Rh, Pd, Ag and Cd) doped LFP.



Supplementary Figure 5. Optimized lattice of TM (TM = La, Hf, Ta, W and Re) doped LFP.



Supplementary Figure 6. Optimized lattice of TM (TM = Os, Ir, Pt, Au and Hg) doped LFP.

Supplementary Table 2. Optimized atomic fractional positions of Sc/Ti doped LFP.

Atoms	x	y	z	Atoms	x	y	z
Li1	-0.007939511	0.013065412	0.010439392	Li1	-0.000746263	0.007088124	0.005103734
Li2	0.500005838	0.488240272	0.00656235	Li2	0.499717656	0.492280484	0.004204963
Li3	-0.007959573	0.012986554	0.491758163	Li3	-0.000732358	0.007264807	0.496237428
Li4	0.499233815	0.4880135	0.491413707	Li4	0.499222615	0.492097175	0.494603294
Fe1	0.975963236	0.282576886	0.248861702	Fe1	0.977178253	0.282049403	0.249057922
Fe2	0.470031341	0.219744199	0.751073989	Fe2	0.475322327	0.219168246	0.750746121
Fe3	0.526230271	0.785067303	0.250429205	Fe3	0.525061397	0.783778651	0.25024854
P1	0.418820318	0.095530964	0.251109162	P1	0.423037488	0.095571045	0.250895806
P2	0.587684098	0.904360643	0.750717277	P2	0.584553692	0.903100619	0.750493082
P3	0.920417741	0.40543989	0.748714343	P3	0.921369466	0.406461679	0.749011134
P4	0.077286725	0.593689779	0.249381876	P4	0.070195478	0.594550529	0.249556052
O1	0.741966086	0.094799109	0.252164937	O1	0.74750535	0.094766795	0.251559062
O2	0.266311833	0.89424463	0.75000501	O2	0.260330981	0.897978716	0.750082139
O3	0.24244909	0.409564767	0.747662708	O3	0.245119147	0.409205109	0.748428355
O4	0.75575511	0.593529881	0.249891014	O4	0.747110261	0.593133827	0.249802407
O5	0.210296018	0.458691043	0.248280183	O5	0.207020073	0.459823596	0.248761951
O6	0.795647491	0.545378999	0.750825345	O6	0.793464587	0.545582885	0.750475519
O7	0.70583181	0.041282649	0.752068441	O7	0.705988922	0.04018781	0.751432584
O8	0.29355687	0.957587347	0.248744662	O8	0.297372231	0.957725546	0.249221483
O9	0.289768578	0.165781369	0.047747358	O9	0.291888651	0.166406257	0.046731406
O10	0.724605955	0.830294744	0.94819139	O10	0.723165774	0.829473897	0.949875927
O11	0.789574383	0.337444873	0.952208288	O11	0.790045321	0.336873494	0.953089686
O12	0.204976961	0.665274949	0.044865848	O12	0.197821192	0.667400455	0.044368971
O13	0.725373254	0.830999338	0.552203512	O13	0.723520182	0.829867076	0.550412902
O14	0.287077371	0.164207033	0.455007359	O14	0.290121	0.165249393	0.455570636
O15	0.205177929	0.664757119	0.454788914	O15	0.197842766	0.667037847	0.455449043
O16	0.787086355	0.338838773	0.544959114	O16	0.788484082	0.337878044	0.544597591
Sc1	0.014770581	0.71860798	0.74992476	Ti1	0.019019708	0.717998495	0.749982274

Supplementary Table 3. Optimized atomic fractional positions of V/Cr doped LFP.

Atoms	x	y	z	Atoms	x	y	z
Li1	-0.003338341	0.004144019	0.002819256	Li1	-0.012051728	0.000639915	0.005312394
Li2	0.499798409	0.499393813	-0.000167681	Li2	0.505973902	0.500492963	0.003468177
Li3	-0.003337527	0.004144117	0.497182169	Li3	-0.012056231	0.000640502	0.494677214
Li4	0.499797877	0.499393788	0.500168051	Li4	0.505974566	0.500493591	0.496537142
Fe1	0.974818884	0.282940542	0.249999388	Fe1	0.972567493	0.283148516	0.249999711
Fe2	0.473385964	0.219559822	0.750000089	Fe2	0.471391481	0.218500901	0.75000054
Fe3	0.525520584	0.780101677	0.250000196	Fe3	0.525811504	0.783091384	0.249994231
P1	0.419901362	0.094747852	0.250000118	P1	0.414134024	0.095901005	0.249998426
P2	0.577978064	0.903892839	0.750000074	P2	0.577245239	0.900916644	0.749994142
P3	0.921317947	0.406073221	0.74999965	P3	0.927437116	0.406542865	0.75000167
P4	0.083172644	0.594012832	0.249999892	P4	0.083267906	0.594642407	0.250007458
O1	0.743955826	0.095529059	0.249999567	O1	0.738353075	0.096545167	0.249998504
O2	0.254374824	0.901104034	0.749999878	O2	0.251236697	0.894146393	0.749998973
O3	0.24488617	0.405197462	0.750000093	O3	0.250727213	0.406116883	0.750001346
O4	0.75936578	0.595452243	0.249999364	O4	0.76004302	0.593769138	0.250004428
O5	0.209300681	0.455864858	0.249999484	O5	0.210055123	0.45626061	0.250000186
O6	0.795217161	0.544620952	0.749999923	O6	0.80928265	0.547612294	0.750006235
O7	0.703101306	0.041627973	0.750000118	O7	0.696332312	0.041920779	0.750002467
O8	0.293322387	0.95634816	0.250000278	O8	0.283502691	0.956799912	0.249994234
O9	0.287480674	0.165795555	0.04524497	O9	0.285184404	0.167501616	0.046267562
O10	0.713999697	0.831223552	0.953021366	O10	0.708424477	0.832022731	0.95453704
O11	0.787818813	0.334728719	0.954203529	O11	0.790437166	0.336237353	0.952700985
O12	0.217192287	0.664847988	0.045051482	O12	0.216984648	0.666938352	0.047854522
O13	0.713999706	0.831223425	0.546978921	O13	0.708416699	0.832031954	0.545437791
O14	0.287481291	0.165795522	0.454755445	O14	0.285184105	0.167499413	0.4537338
O15	0.217192083	0.664847501	0.454949127	O15	0.216980539	0.666931988	0.452168659
O16	0.787818965	0.334729049	0.545795272	O16	0.790437757	0.336238669	0.547299922
V1	0.014476458	0.722659431	0.749999989	Cr1	0.038722131	0.71641606	0.750002252

Supplementary Table 4. Optimized atomic fractional positions of Mn/Fe doped LFP.

Atoms	x	y	z	Atoms	x	y	z
Li1	-0.002649788	0.002226381	0.000757182	Li1	1.09034E-06	0.999999815	-6.97068E-07
Li2	0.501136421	0.498519328	0.000879414	Li2	0.499999003	0.500000186	1.69391E-08
Li3	-0.002650314	0.002226416	0.499242489	Li3	1.06357E-06	0.999999819	0.500000688
Li4	0.501135946	0.498519388	0.499121263	Li4	0.499999001	0.500000164	0.499999954
Fe1	0.974147243	0.281890752	0.250000017	Fe1	0.972159353	0.282293544	0.250000269
Fe2	0.471225014	0.218114877	0.749999957	Fe2	0.027840047	0.717707405	0.749999703
Fe3	0.527779307	0.78263268	0.249999432	Fe3	0.472156248	0.217707912	0.749999875
P1	0.419003729	0.095394678	0.249999832	P1	0.419948915	0.095044525	0.249999853
P2	0.575513439	0.90797103	0.749999612	P2	0.580044173	0.904949446	0.750000029
P3	0.919569795	0.402671327	0.750000292	P3	0.919963776	0.404951976	0.750000209
P4	0.087338256	0.594112422	0.250000255	P4	0.08005265	0.595042097	0.24999973
O1	0.742369371	0.096477465	0.249999573	O1	0.743627709	0.096126642	0.249999573
O2	0.252740736	0.906482322	0.750000589	O2	0.25638366	0.903873038	0.750000433
O3	0.242799472	0.402623782	0.750000019	O3	0.243623695	0.403872831	0.750000211
O4	0.763944787	0.597135511	0.249999733	O4	0.756364971	0.596125861	0.249999784
O5	0.208331856	0.455155122	0.249999506	O5	0.20642014	0.456710365	0.249999687
O6	0.792529251	0.540118929	0.750000577	O6	0.793580569	0.543291133	0.750000278
O7	0.704959934	0.045120136	0.749999972	O7	0.706412281	0.043284401	0.749999514
O8	0.291727409	0.957689545	0.250000605	O8	0.293581655	0.956717143	0.250000475
O9	0.287052165	0.166831569	0.046121783	O9	0.286055599	0.166449521	0.045401854
O10	0.70671044	0.836135906	0.953682432	O10	0.713945069	0.833553794	0.9545895
O11	0.787859304	0.331526202	0.954182635	O11	0.786054816	0.333550394	0.954604701
O12	0.222898661	0.664102701	0.046752889	O12	0.2139431	0.666450626	0.045392396
O13	0.706709818	0.836136396	0.546315877	O13	0.713945018	0.83355347	0.545411759
O14	0.287052254	0.166832116	0.453877531	O14	0.286055541	0.16644991	0.454597074
O15	0.222898215	0.664102152	0.453248206	O15	0.213943534	0.666450418	0.454607226
O16	0.787859124	0.331526227	0.545818019	O16	0.786054442	0.333550645	0.545395792
Mn1	0.020008131	0.717724642	0.750000319	Fe4	0.527842857	0.782292923	0.250000123

Supplementary Table 5. Optimized atomic fractional positions of Co/Ni doped LFP.

Atoms	x	y	z	Atoms	x	y	z
Li1	0.000829175	-0.003421402	-0.001255527	Li1	-0.002645546	-0.004520102	-0.000433927
Li2	0.50026217	0.503401673	-0.001648309	Li2	0.502226413	0.505448291	-0.001962476
Li3	0.000829093	-0.003421391	0.501255642	Li3	-0.002645488	-0.004519813	0.500435435
Li4	0.500262997	0.503401493	0.501646904	Li4	0.502226516	0.505447963	0.501961134
Fe1	0.976121033	0.282176355	0.249999894	Fe1	0.973969607	0.282769527	0.2499997
Fe2	0.476486042	0.218220942	0.74999989	Fe2	0.475805174	0.219074026	0.750000108
Fe3	0.521745122	0.78035703	0.250000304	Fe3	0.523180463	0.780103122	0.250000427
P1	0.421661501	0.095100488	0.250000007	P1	0.41844136	0.095285741	0.250000362
P2	0.575941567	0.904229214	0.750000211	P2	0.574016799	0.901702285	0.750000254
P3	0.921458777	0.404902305	0.750000129	P3	0.924408519	0.407163729	0.749999877
P4	0.081027495	0.596358585	0.249999901	P4	0.084134219	0.595642005	0.249999418
O1	0.745034675	0.096049102	0.249999428	O1	0.74225737	0.096625771	0.250000292
O2	0.253104544	0.904389444	0.750000874	O2	0.249638729	0.89957219	0.749999688
O3	0.245036378	0.403323183	0.75000001	O3	0.247905678	0.404477447	0.750000192
O4	0.757278716	0.59732419	0.249999848	O4	0.760261695	0.596764332	0.24999916
O5	0.205762334	0.457150988	0.250000202	O5	0.206391327	0.455361434	0.249999508
O6	0.79371469	0.54259839	0.749999673	O6	0.800467498	0.546478786	0.749999657
O7	0.704855489	0.042639818	0.749999852	O7	0.69921716	0.041817529	0.750000352
O8	0.294297169	0.956719202	0.25000046	O8	0.2905183	0.955880252	0.250000819
O9	0.288537873	0.167204294	0.045155014	O9	0.28625942	0.1672522	0.045037946
O10	0.709323647	0.832765154	0.955478004	O10	0.70766626	0.831474033	0.956050454
O11	0.788858051	0.332004725	0.95473857	O11	0.789115004	0.334276527	0.954127338
O12	0.215716262	0.667797263	0.045180081	O12	0.2210845	0.666721658	0.045572669
O13	0.709323277	0.832765157	0.544522267	O13	0.707666731	0.831473861	0.543950481
O14	0.288538044	0.167204395	0.454844915	O14	0.286259468	0.167252483	0.454962294
O15	0.215716018	0.667797411	0.454819593	O15	0.221084194	0.666721731	0.454426194
O16	0.78885794	0.332004463	0.545262162	O16	0.789114763	0.334276649	0.545872459
Co1	0.019419898	0.718957534	0.750000011	Ni1	0.021973843	0.719976346	0.750000194

63 **Supplementary Table 6. Optimized atomic fractional positions of Cu/Zn doped**
64 **LFP.**

Atoms	x	y	z	Atoms	x	y	z
Li1	-0.003295236	-0.007648335	-0.003371534	Li1	-0.002729521	-0.000901784	0.001118894
Li2	0.505061017	0.507573446	-0.003503772	Li2	0.501473775	0.501133481	0.001248612
Li3	-0.003299191	-0.007645924	0.503378265	Li3	-0.002728676	-0.000902008	0.498882294
Li4	0.505062579	0.507566589	0.503491718	Li4	0.501474384	0.501133606	0.498749939
Fe1	0.973885672	0.281276695	0.249998791	Fe1	0.974518997	0.2826821	0.249999405
Fe2	0.475834423	0.216951369	0.750003658	Fe2	0.473515293	0.218932343	0.749999739
Fe3	0.518428752	0.782294176	0.250002328	Fe3	0.527612158	0.78169875	0.249999969
P1	0.417244329	0.095606942	0.250005067	P1	0.419362646	0.095395697	0.2499997
P2	0.569787229	0.905255219	0.750003549	P2	0.576581412	0.903488603	0.749999403
P3	0.924305014	0.403250204	0.749996239	P3	0.921951325	0.406040192	0.749999881
P4	0.085946667	0.595702918	0.249995887	P4	0.082782834	0.595545359	0.250000794
O1	0.740184519	0.097439103	0.250004006	O1	0.743013209	0.096109468	0.249999146
O2	0.246372725	0.906548955	0.7500024	O2	0.252735123	0.900141236	0.750000024
O3	0.24765948	0.400399271	0.74999676	O3	0.245270341	0.405403801	0.750000037
O4	0.762675633	0.59933824	0.24999764	O4	0.759257622	0.596012531	0.249999316
O5	0.201978997	0.454384606	0.24999661	O5	0.208310061	0.45677994	0.249999735
O6	0.800899094	0.541467139	0.749997438	O6	0.795402665	0.544633739	0.750000073
O7	0.700636829	0.045488994	0.750002925	O7	0.701434109	0.042390686	0.749999938
O8	0.287173717	0.956642378	0.25000455	O8	0.291533962	0.956976306	0.250000289
O9	0.285871698	0.168146296	0.046194537	O9	0.287433869	0.167227259	0.045290795
O10	0.695651855	0.837457638	0.959039463	O10	0.711013072	0.832079662	0.953999599
O11	0.790053066	0.329746773	0.953634472	O11	0.788472738	0.334265105	0.954371228
O12	0.227212022	0.666566708	0.049132973	O12	0.216814724	0.666583408	0.0450037
O13	0.695652355	0.837456041	0.540969258	O13	0.711012962	0.832080013	0.545998763
O14	0.285871521	0.168145578	0.453814298	O14	0.287434205	0.167227677	0.454708714
O15	0.227215189	0.666566757	0.450859274	O15	0.216812813	0.666583079	0.454998574
O16	0.790050198	0.329748468	0.546358834	O16	0.788473058	0.334265203	0.545628278
Cu1	0.045879823	0.714273762	0.749994375	Zn1	0.021760813	0.71699455	0.750003173

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66 **Supplementary Table 7. Optimized atomic fractional positions of Y/Zr doped**
67 **LFP.**

Atoms	x	y	z	Atoms	x	y	z
Li1	-0.012761377	0.019814615	0.009149475	Li1	-0.008386668	0.016450539	0.009556058
Li2	0.500590928	0.480612217	0.00477087	Li2	0.500495833	0.481561015	0.007683236
Li3	-0.012767453	0.019833798	0.490884327	Li3	-0.008379192	0.016450862	0.490483567
Li4	0.500462566	0.480567588	0.495280738	Li4	0.50045424	0.481556289	0.492283452
Fe1	0.975762532	0.282070902	0.24991487	Fe1	0.977037107	0.281531619	0.250173039
Fe2	0.462653146	0.217861134	0.750099043	Fe2	0.467258413	0.216605755	0.749778764
Fe3	0.524067179	0.790950403	0.249997068	Fe3	0.526957571	0.789331467	0.249995074
P1	0.415983092	0.096884629	0.250018026	P1	0.420405106	0.096146047	0.249982856
P2	0.579210409	0.914118079	0.749989664	P2	0.586923754	0.91024333	0.750003593
P3	0.915653523	0.398514846	0.749958617	P3	0.922436869	0.400185448	0.750001841
P4	0.097834135	0.58848646	0.250006186	P4	0.07306688	0.590657996	0.249998773
O1	0.737612146	0.09686715	0.249978509	O1	0.745211307	0.096340263	0.250024252
O2	0.258948014	0.908023939	0.75001454	O2	0.262557077	0.903116514	0.749967885
O3	0.236222288	0.405699341	0.750010058	O3	0.246301358	0.406816815	0.749977477
O4	0.778997916	0.594783782	0.249950532	O4	0.750405301	0.591330757	0.25000943
O5	0.218391795	0.453510547	0.249987481	O5	0.2069763	0.45833873	0.249971948
O6	0.784760383	0.534525878	0.749986027	O6	0.795511372	0.538329239	0.750014029
O7	0.706073053	0.04716842	0.749998907	O7	0.707365601	0.045072196	0.750020796
O8	0.289577848	0.961370082	0.250015669	O8	0.294990688	0.959875287	0.250010603
O9	0.286621824	0.165442553	0.047977051	O9	0.289613644	0.164533931	0.047993495
O10	0.707325686	0.840368621	0.94824206	O10	0.724555222	0.839249459	0.948884051
O11	0.787548828	0.332330004	0.953075234	O11	0.790207589	0.335318664	0.952863794
O12	0.232931149	0.657355046	0.049106938	O12	0.203245095	0.66274926	0.049228594
O13	0.707301139	0.84034743	0.551772651	O13	0.72459303	0.839274497	0.551122079
O14	0.286642648	0.165418901	0.451992723	O14	0.289692235	0.164547582	0.452024731
O15	0.232877049	0.657355035	0.450887869	O15	0.203262375	0.662719026	0.450801732
O16	0.787570829	0.332373257	0.546922332	O16	0.79023652	0.335297089	0.547151378
Y1	0.013908701	0.717345347	0.750012543	Zr1	0.017005351	0.71637033	0.749993484

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Supplementary Table 8. Optimized atomic fractional positions of Nb/Mo doped LFP.

Atoms	x	y	z	Atoms	x	y	z
Li1	-0.004029263	0.012745646	0.004561439	Li1	-0.008436948	0.012794776	0.009694715
Li2	0.502641071	0.491144169	0.002563136	Li2	0.501154801	0.493316819	0.002131804
Li3	-0.003988079	0.012821301	0.494870953	Li3	-0.008330871	0.012828588	0.492408095
Li4	0.502956659	0.491204335	0.49783769	Li4	0.500272559	0.49282308	0.496538959
Fe1	0.976545112	0.281312242	0.250139028	Fe1	0.973691493	0.282123837	0.249018576
Fe2	0.471641273	0.218935938	0.749676488	Fe2	0.469847904	0.220577469	0.751217676
Fe3	0.521053259	0.782902341	0.249943675	Fe3	0.520669328	0.780768142	0.250117306
P1	0.420356935	0.09537666	0.249679882	P1	0.417044488	0.095031541	0.251196865
P2	0.577806128	0.909602293	0.749791583	P2	0.583728054	0.905346277	0.750612934
P3	0.921783504	0.401855104	0.750326457	P3	0.920623094	0.405916002	0.748763304
P4	0.081603673	0.589511802	0.250240538	P4	0.084096175	0.590013522	0.24926718
O1	0.744343091	0.095623781	0.24901644	O1	0.74065296	0.095407514	0.251920614
O2	0.254114726	0.909746427	0.750065741	O2	0.259970083	0.901668496	0.750189544
O3	0.245033922	0.404632839	0.751089176	O3	0.242768676	0.408003557	0.748085582
O4	0.75955323	0.592107165	0.250003132	O4	0.762603894	0.593042695	0.249336169
O5	0.211443302	0.454833254	0.250848294	O5	0.213365173	0.454381654	0.248557288
O6	0.792325641	0.538718835	0.749279754	O6	0.792325649	0.545218513	0.750480188
O7	0.707596897	0.043750954	0.74931858	O7	0.705355318	0.041462963	0.751672747
O8	0.29334745	0.959015659	0.250518408	O8	0.290766732	0.957412623	0.249664831
O9	0.288832464	0.165141167	0.046205027	O9	0.287254157	0.165203743	0.046980904
O10	0.707793382	0.836082054	0.952204779	O10	0.717874864	0.831181719	0.952024666
O11	0.789358744	0.333650328	0.954062499	O11	0.78805878	0.33715489	0.952171886
O12	0.216513599	0.661171767	0.048330827	O12	0.219929735	0.660649709	0.045102268
O13	0.707632315	0.835842192	0.547751238	O13	0.718209662	0.8317314	0.54836615
O14	0.29033544	0.165660053	0.453235628	O14	0.285447733	0.164264989	0.455542246
O15	0.216327082	0.66154866	0.451647949	O15	0.219626426	0.660438348	0.454187573
O16	0.791061689	0.332931254	0.546703035	O16	0.78607994	0.338357456	0.544981297
Nb1	0.01601673	0.722131785	0.750088635	Mo1	0.015350117	0.722879681	0.749768643

Supplementary Table 9. Optimized atomic fractional positions of Tc/Ru doped LFP.

Atoms	x	y	z	Atoms	x	y	z
Li1	0.000239396	0.005413477	0.002615341	Li1	-0.002249486	0.002999489	0.002622063
Li2	0.500345925	0.498693373	0.998822166	Li2	0.500287215	0.502688355	-0.002840162
Li3	0.000242847	0.005413796	0.497385634	Li3	-0.002249404	0.002999691	0.497379198
Li4	0.500345495	0.498694681	0.501176705	Li4	0.500287794	0.502688145	0.502838658
Fe1	0.974829641	0.282037349	0.250000584	Fe1	0.97292779	0.283030875	0.249999477
Fe2	0.474773584	0.219942966	0.750000064	Fe2	0.473086717	0.220698446	0.750000199
Fe3	0.515963355	0.779021991	0.250001456	Fe3	0.522081021	0.77708878	0.250000316
P1	0.422051827	0.095003273	0.250003684	P1	0.419480817	0.094733676	0.250000385
P2	0.578969938	0.905236941	0.750000452	P2	0.576337732	0.903144204	0.750000348
P3	0.921013412	0.406046036	0.75000406	P3	0.920793135	0.407723648	0.749999697
P4	0.079820507	0.59100147	0.249998161	P4	0.087647027	0.591461271	0.249999607
O1	0.746040995	0.095424962	0.249996125	O1	0.743205635	0.095824846	0.249999822
O2	0.255040485	0.907487056	0.750001914	O2	0.251840285	0.906171183	0.750000828
O3	0.24437971	0.405691296	0.74999672	O3	0.243530438	0.405603592	0.74999966
O4	0.757545125	0.593362365	0.250002653	O4	0.765310606	0.594510616	0.249999462
O5	0.210216233	0.454724383	0.249998094	O5	0.211873968	0.452311997	0.24999901
O6	0.789342686	0.543368579	0.749999003	O6	0.789577664	0.546177809	0.750000507
O7	0.707413003	0.040946978	0.749999641	O7	0.703384329	0.040668657	0.750000354
O8	0.295135815	0.957710797	0.250000045	O8	0.292993017	0.95619021	0.25000103
O9	0.289666139	0.165939764	0.044950755	O9	0.287272636	0.166257764	0.044685673
O10	0.710874718	0.831182925	0.954767167	O10	0.708271043	0.830344126	0.957004947
O11	0.788248616	0.33488767	0.954338947	O11	0.78673418	0.335433422	0.954005934
O12	0.216913975	0.662794436	0.045553674	O12	0.228371889	0.660652111	0.044127968
O13	0.710879879	0.831183205	0.545232003	O13	0.708270577	0.830344107	0.542995452
O14	0.289666833	0.16593896	0.455048909	O14	0.287273108	0.166258048	0.455315068
O15	0.216913246	0.662794574	0.454442277	O15	0.228371558	0.660651788	0.455871562
O16	0.788247756	0.334883639	0.545665176	O16	0.78673447	0.335434022	0.545992842
Tc1	0.014878836	0.725173063	0.749998599	Ru1	0.008554216	0.727909127	0.750000107

Supplementary Table 10. Optimized atomic fractional positions of Rh/Pd doped LFP.

Atoms	x	y	z	Atoms	x	y	z
Li1	-0.010702471	0.000577919	0.001954987	Li1	-0.009059304	-0.000235094	-0.001391772
Li2	0.507947575	0.503694545	-0.002225708	Li2	0.509575666	0.50364762	-0.004089245
Li3	-0.010702118	0.000578187	0.498045455	Li3	-0.009041009	-0.000230082	0.50142329
Li4	0.507949107	0.503694254	0.502223512	Li4	0.509550512	0.503637058	0.504072012
Fe1	0.97116192	0.281337143	0.250000357	Fe1	0.972942343	0.279408599	0.250001735
Fe2	0.470332069	0.218689951	0.750000142	Fe2	0.470191426	0.216750387	0.750009058
Fe3	0.520712153	0.781290677	0.24999999	Fe3	0.518513981	0.783304102	0.25001478
P1	0.413123601	0.095048681	0.249999869	P1	0.413940595	0.095424858	0.24998995
P2	0.569661198	0.904966909	0.749999913	P2	0.563531214	0.912142201	0.750003741
P3	0.926199745	0.404413495	0.75000037	P3	0.923947036	0.39816195	0.749996114
P4	0.095237921	0.59106456	0.250000272	P4	0.100349975	0.590487583	0.249989855
O1	0.736284054	0.096495135	0.250000218	O1	0.735982208	0.09781485	0.250010097
O2	0.244174624	0.906163437	0.750000305	O2	0.241512654	0.917721176	0.749998035
O3	0.24819307	0.40346397	0.750000054	O3	0.245603374	0.39736395	0.749999608
O4	0.774126321	0.596517197	0.250000179	O4	0.780352007	0.599623779	0.249978387
O5	0.210801675	0.450874033	0.249999606	O5	0.205881722	0.449449963	0.249993347
O6	0.800839422	0.543448302	0.749999298	O6	0.796259977	0.533872491	0.749982644
O7	0.697095386	0.044371685	0.750000884	O7	0.700615025	0.049275002	0.750005354
O8	0.28256997	0.956154612	0.249999809	O8	0.283161168	0.957924309	0.250008068
O9	0.28406274	0.166735601	0.046518448	O9	0.284449124	0.167423197	0.047668643
O10	0.694214618	0.836472867	0.958115135	O10	0.683303362	0.844247176	0.958890831
O11	0.789954362	0.333035116	0.952671837	O11	0.790960152	0.326160823	0.953133681
O12	0.241304467	0.661184517	0.050011335	O12	0.251220523	0.659212857	0.052561858
O13	0.694213734	0.83647399	0.541883325	O13	0.683300734	0.844233825	0.541162157
O14	0.284062435	0.166735631	0.453481234	O14	0.284449471	0.167424591	0.452350024
O15	0.241304412	0.661183898	0.449990007	O15	0.251221672	0.659217357	0.447391815
O16	0.789954152	0.333034377	0.547329697	O16	0.790955756	0.326158668	0.546851973
Rh1	0.025923834	0.722299315	0.749999482	Pd1	0.026328613	0.720376807	0.749993973

78 **Supplementary Table 11. Optimized atomic fractional positions of Ag/Cd doped**
79 **LFP.**

Atoms	x	y	z	Atoms	x	y	z
Li1	-0.007724491	0.000674064	-0.004467523	Li1	-0.005976991	0.007607787	0.000603983
Li2	0.506763466	0.504923467	-0.008545892	Li2	0.501464516	0.494017646	-0.000891034
Li3	-0.007724598	0.000673994	0.504467623	Li3	-0.005974995	0.007608427	0.499399793
Li4	0.506764564	0.504924512	0.508544709	Li4	0.501464386	0.494017491	0.500889268
Fe1	0.980539947	0.277575392	0.250000803	Fe1	0.973123218	0.280411451	0.249999947
Fe2	0.473886062	0.213690631	0.749999996	Fe2	0.466821964	0.217227819	0.750000377
Fe3	0.514188737	0.783968074	0.249999354	Fe3	0.526307819	0.78535198	0.250000315
P1	0.417761813	0.095302656	0.24999998	P1	0.416766979	0.095945029	0.250000397
P2	0.556751431	0.919866911	0.749999793	P2	0.569981368	0.91480164	0.75000043
P3	0.92226666	0.389345944	0.750000744	P3	0.916529252	0.397247526	0.749999613
P4	0.10628682	0.591700634	0.249999554	P4	0.100125033	0.590706748	0.249999152
O1	0.738158324	0.097966558	0.250000403	O1	0.738979265	0.097084097	0.250000343
O2	0.240987982	0.934730013	0.749999852	O2	0.248617692	0.918136984	0.750000171
O3	0.243542775	0.389604756	0.750000609	O3	0.238445929	0.399429669	0.749999432
O4	0.787801209	0.605639237	0.249999703	O4	0.779654687	0.599800466	0.249999547
O5	0.198657361	0.449800079	0.250001356	O5	0.210332191	0.451429508	0.249998955
O6	0.787354539	0.519794737	0.750000256	O6	0.782326114	0.531529385	0.749999217
O7	0.707903839	0.053067865	0.749999816	O7	0.705586412	0.049226882	0.750000258
O8	0.284073908	0.960582812	0.249999641	O8	0.288681486	0.959764765	0.25000113
O9	0.288334605	0.168373281	0.048547976	O9	0.286214852	0.1671285	0.047473144
O10	0.670537909	0.851492436	0.960590001	O10	0.694054493	0.843222506	0.954598379
O11	0.795427429	0.315518585	0.953928434	O11	0.78812615	0.326710206	0.953783071
O12	0.261302872	0.657133747	0.05287484	O12	0.245781174	0.658273134	0.050517213
O13	0.670538004	0.851492326	0.539409902	O13	0.694054619	0.843222221	0.545402808
O14	0.288334356	0.16837313	0.451452169	O14	0.286214963	0.167128918	0.45252717
O15	0.261303089	0.657135081	0.447123032	O15	0.24578137	0.658273091	0.449480908
O16	0.795427569	0.315518041	0.5460735	O16	0.788126112	0.326710057	0.546216591
Ag1	0.010553796	0.721131042	0.749999377	Cd1	0.018389921	0.717986069	0.749999433

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Supplementary Table 12. Optimized atomic fractional positions of La/Hf doped LFP.

Atoms	x	y	z	Atoms	x	y	z
Li1	-0.019590399	0.025911518	0.005532938	Li1	-0.012910483	0.019919962	0.015635471
Li2	0.517303555	0.473749301	0.005039989	Li2	0.499505077	0.479314341	0.009661137
Li3	-0.01960212	0.025879102	0.494465285	Li3	-0.013551828	0.019640802	0.48719024
Li4	0.516909835	0.473621169	0.49521164	Li4	0.498626563	0.479703046	0.48649155
Fe1	0.984956937	0.280238553	0.250017722	Fe1	0.977851606	0.282145793	0.248565911
Fe2	0.46497397	0.217773992	0.749973353	Fe2	0.46510567	0.217712583	0.751638142
Fe3	0.488124146	0.801827022	0.250005872	Fe3	0.531598762	0.789598845	0.250822018
P1	0.410953686	0.100788869	0.250006931	P1	0.418229257	0.095924316	0.251416912
P2	0.556489032	0.924348465	0.750003224	P2	0.59425224	0.905147544	0.751129381
P3	0.925172441	0.390321419	0.749976918	P3	0.925522866	0.402352886	0.748362916
P4	0.12476724	0.58032556	0.249963541	P4	0.06619605	0.593264837	0.249193183
O1	0.730980242	0.099419611	0.250026809	O1	0.742474593	0.095718822	0.252625987
O2	0.236842815	0.924542813	0.749997986	O2	0.272063471	0.890874675	0.74998415
O3	0.243929636	0.399443604	0.749926191	O3	0.248475846	0.40952325	0.746718449
O4	0.80818114	0.584649228	0.249774317	O4	0.744368127	0.591293879	0.250232235
O5	0.240736351	0.448776731	0.250030695	O5	0.204928444	0.462094538	0.247172028
O6	0.792027633	0.520558212	0.749960447	O6	0.805467831	0.543262697	0.751600533
O7	0.700016989	0.052108078	0.749962772	O7	0.706072035	0.0413662	0.752887092
O8	0.272655768	0.969942426	0.249993572	O8	0.292559303	0.958971734	0.248179803
O9	0.287037757	0.168872699	0.04764023	O9	0.291324896	0.165200573	0.049472441
O10	0.671645934	0.850675186	0.950162869	O10	0.735788635	0.833367399	0.947332093
O11	0.796626752	0.324948022	0.954144942	O11	0.792865924	0.337999017	0.951027344
O12	0.260467384	0.649651592	0.048840926	O12	0.19081951	0.666699989	0.04675359
O13	0.671664179	0.850623522	0.549827394	O13	0.737353592	0.834346099	0.553638135
O14	0.286986701	0.168898265	0.452330385	O14	0.287598971	0.16313463	0.454027935
O15	0.260158681	0.649677815	0.451214742	O15	0.191581231	0.665433883	0.453012909
O16	0.79652374	0.324897835	0.545862899	O16	0.790117499	0.340113542	0.545289021
La1	-0.006940047	0.717529395	0.750105423	Hf1	0.015714288	0.715874123	0.749939407

Supplementary Table 13. Optimized atomic fractional positions of Ta/W doped LFP.

Atoms	x	y	z	Atoms	x	y	z
Li1	-0.056105674	0.005772322	0.018802948	Li1	-0.009645784	0.014601985	0.011182391
Li2	0.513315449	0.489362	0.013888604	Li2	0.49902656	0.492050415	0.003566466
Li3	-0.065045171	0.027406599	0.508078755	Li3	-0.00921413	0.014604431	0.489816829
Li4	0.522849726	0.492228757	0.496783212	Li4	0.498550132	0.49143042	0.496568428
Fe1	-0.020496125	0.286244652	0.249785793	Fe1	0.973667024	0.283216936	0.250300273
Fe2	0.466335631	0.211009776	0.744832149	Fe2	0.469978322	0.22007199	0.750439056
Fe3	0.551619239	0.78662704	0.242115146	Fe3	0.520611365	0.781064379	0.249306824
P1	0.411204041	0.098029262	0.240347189	P1	0.417907743	0.095036197	0.250529814
P2	0.486661791	0.885266603	0.748661789	P2	0.587636366	0.903734657	0.750087154
P3	0.942788759	0.409167751	0.752010879	P3	0.922508384	0.406510493	0.749884613
P4	0.091872924	0.589856244	0.252569222	P4	0.077074032	0.590412042	0.249366866
O1	0.735793453	0.106505612	0.252991509	O1	0.74234218	0.0954788	0.250401633
O2	0.194427541	0.915670793	0.638647236	O2	0.262691348	0.897842599	0.750651498
O3	0.263690102	0.406951825	0.747518893	O3	0.245349891	0.40852697	0.750195053
O4	0.771520613	0.583276783	0.252169812	O4	0.755015487	0.591703484	0.247933095
O5	0.22653914	0.455853295	0.26808091	O5	0.210676362	0.456075141	0.250940039
O6	0.839648415	0.553861358	0.746986356	O6	0.796986119	0.546732575	0.74911682
O7	0.643886806	0.023199797	0.774874084	O7	0.705152446	0.040101162	0.750150155
O8	0.305896433	0.956769365	0.207738186	O8	0.292246959	0.957410145	0.251230322
O9	0.287823391	0.177912214	0.0491303	O9	0.286772993	0.163914988	0.046014709
O10	0.833325779	0.816505614	0.003672353	O10	0.725790797	0.830128836	0.950824608
O11	0.801317573	0.34540502	0.958038849	O11	0.787358614	0.339738234	0.953264018
O12	0.232228234	0.647170976	0.034334122	O12	0.212935241	0.661068221	0.045276212
O13	0.699190318	0.813237117	0.574475014	O13	0.725091203	0.830557855	0.549049469
O14	0.275173778	0.16163755	0.450749749	O14	0.287263605	0.164374011	0.454321156
O15	0.211623496	0.675294658	0.445686174	O15	0.209759241	0.662412537	0.453259562
O16	0.797181212	0.338230963	0.553799159	O16	0.787040092	0.339506011	0.546797609
Ta1	0.035733107	0.74154606	0.773231619	W1	0.019427387	0.721694489	0.749525342

Supplementary Table 14. Optimized atomic fractional positions of Re/Os doped LFP.

Atoms	x	y	z	Atoms	x	y	z
Li1	-0.001473993	0.00931462	0.004541138	Li1	-0.001371384	0.004699157	0.002980793
Li2	0.499346431	0.495961348	0.000417363	Li2	0.499888688	0.502110114	-0.002584358
Li3	-0.001712651	0.009515356	0.494447754	Li3	-0.001370351	0.004699672	0.497022055
Li4	0.49959019	0.496031135	0.500265981	Li4	0.499888531	0.502109896	0.502583117
Fe1	0.975086953	0.28194426	0.250730428	Fe1	0.973227682	0.283063801	0.249999437
Fe2	0.475104904	0.220337258	0.74916643	Fe2	0.474323505	0.220771674	0.750000252
Fe3	0.514661468	0.779693034	0.250074481	Fe3	0.519514206	0.777233855	0.250000171
P1	0.42137209	0.094772341	0.24922221	P1	0.420387218	0.094828369	0.250000657
P2	0.582914175	0.903513432	0.749810488	P2	0.577478818	0.902642546	0.750000134
P3	0.922561816	0.407107448	0.750796194	P3	0.922261834	0.408090053	0.749999408
P4	0.075276845	0.59034223	0.250245717	P4	0.084028858	0.590418701	0.249999465
O1	0.745906003	0.094836222	0.248792018	O1	0.74455738	0.095376404	0.250000057
O2	0.257340491	0.904612036	0.750454346	O2	0.251832653	0.907100864	0.750000579
O3	0.246071131	0.407854305	0.751185316	O3	0.24519286	0.406326986	0.749998983
O4	0.752918905	0.591930573	0.249845117	O4	0.761682496	0.593013666	0.249999603
O5	0.210574218	0.455605784	0.251353689	O5	0.212344231	0.452385477	0.249998916
O6	0.792143211	0.545974068	0.748924678	O6	0.791159554	0.547096786	0.750000489
O7	0.708115255	0.039286027	0.748865541	O7	0.705301946	0.039568239	0.750000283
O8	0.294442656	0.957261709	0.250740418	O8	0.29349905	0.956500735	0.250001395
O9	0.289127095	0.164581075	0.043907933	O9	0.288641052	0.166069799	0.044656937
O10	0.717239244	0.829342863	0.95431235	O10	0.70766243	0.8292442	0.957823233
O11	0.788176026	0.338302255	0.955428888	O11	0.787596048	0.33651236	0.953778318
O12	0.211180966	0.66276497	0.045239663	O12	0.224403453	0.660036575	0.044138797
O13	0.716441804	0.828930526	0.545795294	O13	0.707662133	0.829244192	0.542176756
O14	0.290054147	0.165542779	0.453900628	O14	0.288641367	0.166070113	0.455344293
O15	0.210567575	0.663399687	0.454423002	O15	0.224403269	0.660036265	0.455860424
O16	0.789133504	0.337077547	0.547145014	O16	0.787595992	0.336513018	0.546219992
Re1	0.017839518	0.724165115	0.74996793	Os1	0.009566458	0.728236485	0.749999824

Supplementary Table 15. Optimized atomic fractional positions of Ir/Pt doped LFP.

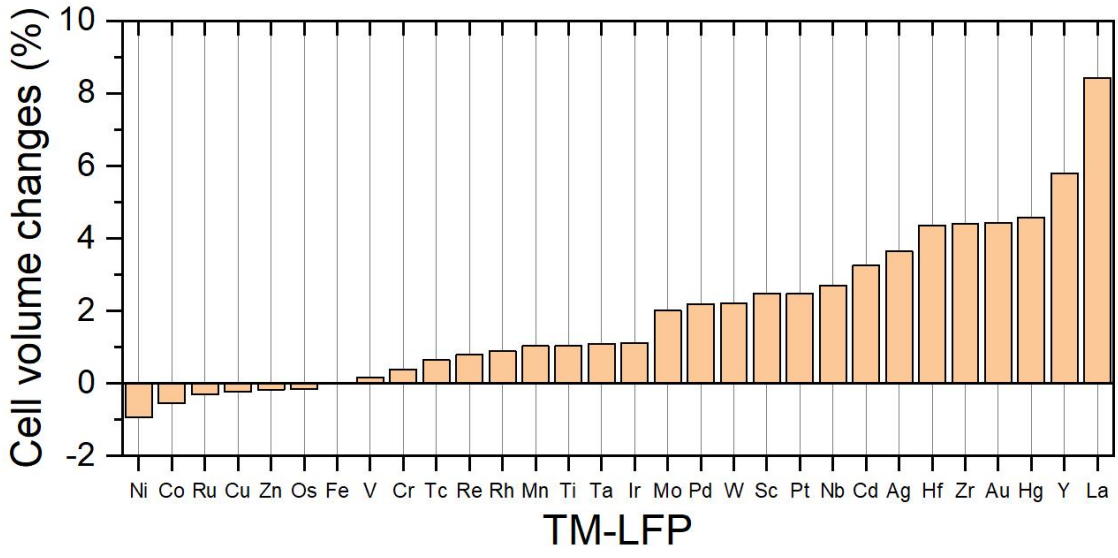
Atoms	x	y	z	Atoms	x	y	z
Li1	-0.013507463	0.002727379	0.004969361	Li1	-0.010126822	0.003289753	0.000842524
Li2	0.507647104	0.503111206	-0.00114319	Li2	0.508784787	0.501211248	-0.002994797
Li3	-0.013507988	0.002727294	0.495029899	Li3	-0.010126641	0.003289692	0.499156842
Li4	0.507647546	0.503111273	0.501141138	Li4	0.508785129	0.501210869	0.502994099
Fe1	0.970015891	0.282024005	0.250000559	Fe1	0.973005368	0.279666778	0.250000722
Fe2	0.469320703	0.218667843	0.750000116	Fe2	0.469603579	0.21738226	0.750000151
Fe3	0.522027124	0.782708156	0.250000995	Fe3	0.516879289	0.783782172	0.250000328
P1	0.411438743	0.095661406	0.2500003	P1	0.414240597	0.095514085	0.249999791
P2	0.573439084	0.902738205	0.750001481	P2	0.565357776	0.91194596	0.750000255
P3	0.928245773	0.404942859	0.750000358	P3	0.924756971	0.398654347	0.750000279
P4	0.091452464	0.590291619	0.249998081	P4	0.098598851	0.5891086	0.249999896
O1	0.735177543	0.096758949	0.250000724	O1	0.736615636	0.097040682	0.25000034
O2	0.245994714	0.902449651	0.749999201	O2	0.242267285	0.917378603	0.749999217
O3	0.250274081	0.404432822	0.750000542	O3	0.246367546	0.399196335	0.749999118
O4	0.770485837	0.594082486	0.249999205	O4	0.77899115	0.597448227	0.250000042
O5	0.211980104	0.451433428	0.249999472	O5	0.209100568	0.449633933	0.249999594
O6	0.805119574	0.545349511	0.750000527	O6	0.795214907	0.534581419	0.750000025
O7	0.695602439	0.042812713	0.749998698	O7	0.701559987	0.048213014	0.750000811
O8	0.280050042	0.956868439	0.250000924	O8	0.282979697	0.958405439	0.249999644
O9	0.283480012	0.166955577	0.046545319	O9	0.285452059	0.167044256	0.047368567
O10	0.698791014	0.83498803	0.958030246	O10	0.685266468	0.843005185	0.958353968
O11	0.790078921	0.334901906	0.951964623	O11	0.791863339	0.327627393	0.953173075
O12	0.236879607	0.661255838	0.050136656	O12	0.249335622	0.65819672	0.051786501
O13	0.698798029	0.834984736	0.541977769	O13	0.685267451	0.843005328	0.54164682
O14	0.283479927	0.166955831	0.453453771	O14	0.285451632	0.167044194	0.452630859
O15	0.236882456	0.661257387	0.449855023	O15	0.249335964	0.658196522	0.448213258
O16	0.790078375	0.334902579	0.548035981	O16	0.791862185	0.32762712	0.546828074
Ir1	0.032628323	0.720898877	0.750002229	Pt1	0.023309598	0.721299868	0.750000008

Supplementary Table 16. Optimized atomic fractional positions of Au/Hg doped LFP.

Atoms	x	y	z	Atoms	x	y	z
Li1	-0.003156926	0.002191393	-0.003991562	Li1	-0.005898819	0.009355256	-0.000262384
Li2	0.492476528	0.499860206	-0.014118541	Li2	0.499217585	0.491684638	-0.00322191
Li3	-0.003156921	0.002191262	0.503991229	Li3	-0.005897871	0.009355177	0.500261691
Li4	0.492472393	0.499859601	0.514121784	Li4	0.499200854	0.491682057	0.50323357
Fe1	0.978235881	0.277139205	0.250000212	Fe1	0.973358722	0.279175788	0.249999439
Fe2	0.473055413	0.211959887	0.749999926	Fe2	0.466052718	0.215906587	0.750000846
Fe3	0.519598821	0.78404619	0.249999691	Fe3	0.523771392	0.787528277	0.249998637
P1	0.420058366	0.095749481	0.24999993	P1	0.416774067	0.09646087	0.249999534
P2	0.562055067	0.921100786	0.749999654	P2	0.567166212	0.918322354	0.749998256
P3	0.916595241	0.387747661	0.750000363	P3	0.915722723	0.393669767	0.750000188
P4	0.104287499	0.592933305	0.249999532	P4	0.104066292	0.589519086	0.249999629
O1	0.739741792	0.097547073	0.249999833	O1	0.737907523	0.097420235	0.249999974
O2	0.248062299	0.940982473	0.7499995	O2	0.247120135	0.926122155	0.749997188
O3	0.237297796	0.38962453	0.750000161	O3	0.236506636	0.397415919	0.749999846
O4	0.788527811	0.610439542	0.249999762	O4	0.786406214	0.601506534	0.249997722
O5	0.194555483	0.451028883	0.249999612	O5	0.210241964	0.450658573	0.250000559
O6	0.77564483	0.517304048	0.750000032	O6	0.776810607	0.526043111	0.749999371
O7	0.715126398	0.052486375	0.749999654	O7	0.70788035	0.050863253	0.749999752
O8	0.288054046	0.961693459	0.249999985	O8	0.287463409	0.961438465	0.249998171
O9	0.290545658	0.169080078	0.049095166	O9	0.287180266	0.167605759	0.048114756
O10	0.672947255	0.851208295	0.960318951	O10	0.685566927	0.846978327	0.95580382
O11	0.793682986	0.314252214	0.95392431	O11	0.789347655	0.323460511	0.953726856
O12	0.263139179	0.65745961	0.054110292	O12	0.256149792	0.656430433	0.052850498
O13	0.672947595	0.851208208	0.53968049	O13	0.685566342	0.846978206	0.544194127
O14	0.290545608	0.169080163	0.450904695	O14	0.287180095	0.167605663	0.451883217
O15	0.263139136	0.65745961	0.445888632	O15	0.256144019	0.656429982	0.447149117
O16	0.793682807	0.314251745	0.546077085	O16	0.789348127	0.323458952	0.546277162
Au1	0.019837938	0.72011472	0.749999632	Hg1	0.019646041	0.71692407	0.750000378

Supplementary Table 17. Lattice parameters of $LiFePO_4$ before and after doping by 3d, 4d and 5d transition metals.

Materials	Notes	a (Å)	b (Å)	c (Å)	Cell volume (Å^3)
$LiFePO_4$	Ours	10.37	6.04	4.73	296.26
$LiFePO_4$	Exp.[5]	10.33	6.01	4.69	291.17
$LiFePO_4$	Cal.[6]	10.49	5.92	4.75	294.73
$LiFePO_4$	Cal.[7]	10.35	6.03	4.72	294.58
Sc-$LiFePO_4$	Ours	10.46	6.11	4.76	305.05
Ti-$LiFePO_4$	Ours	10.44	6.07	4.74	300.79
V-$LiFePO_4$	Ours	10.38	6.04	4.74	298.18
Cr-$LiFePO_4$	Ours	10.31	6.10	4.74	298.87
Mn-$LiFePO_4$	Ours	10.41	6.07	4.75	300.76
Co-$LiFePO_4$	Ours	10.35	6.02	4.74	296.05
Ni-$LiFePO_4$	Ours	10.29	6.03	4.74	294.91
Cu-$LiFePO_4$	Ours	10.30	6.05	4.75	297.02
Zn-$LiFePO_4$	Ours	10.35	6.03	4.74	297.18
Y-$LiFePO_4$	Ours	10.64	6.17	4.79	314.93
Zr-$LiFePO_4$	Ours	10.61	6.17	4.74	310.82
Nb-$LiFePO_4$	Ours	10.54	6.10	4.75	305.73
Mo-$LiFePO_4$	Ours	10.47	6.09	4.75	303.67
Tc-$LiFePO_4$	Ours	10.44	6.04	4.74	299.62
Ru-$LiFePO_4$	Ours	10.35	6.03	4.75	296.8
Rh-$LiFePO_4$	Ours	10.33	6.09	4.76	300.33
Pd-$LiFePO_4$	Ours	10.42	6.10	4.77	304.21
Ag-$LiFePO_4$	Ours	10.56	6.08	4.79	308.56
Cd-$LiFePO_4$	Ours	10.52	6.11	4.77	307.37
La-$LiFePO_4$	Ours	10.92	6.14	4.81	322.78
Hf-$LiFePO_4$	Ours	10.58	6.17	4.75	310.66
Ta-$LiFePO_4$	Ours	10.33	6.10	4.77	300.96
W-$LiFePO_4$	Ours	10.49	6.10	4.74	304.27
Re-$LiFePO_4$	Ours	10.45	6.05	4.73	300.03
Os-$LiFePO_4$	Ours	10.37	6.04	4.74	297.24
Ir-$LiFePO_4$	Ours	10.34	6.11	4.75	301.03
Pt-$LiFePO_4$	Ours	10.48	6.10	4.77	305.07
Au-$LiFePO_4$	Ours	10.59	6.09	4.80	310.90
Hg-$LiFePO_4$	Ours	10.60	6.12	4.79	311.33



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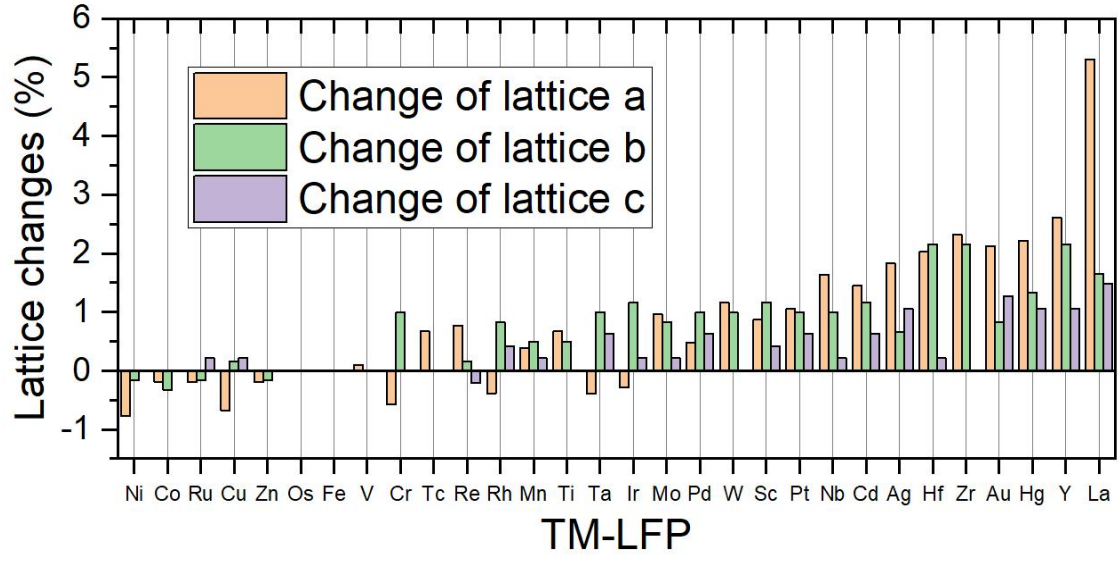
101 **Supplementary Figure 7. Order of cell volume changes of TM-LFP models.**



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103 **Supplementary Figure 8. Lattice changes of TM-LFP models according to the**

104 **order of cell volume changes.**

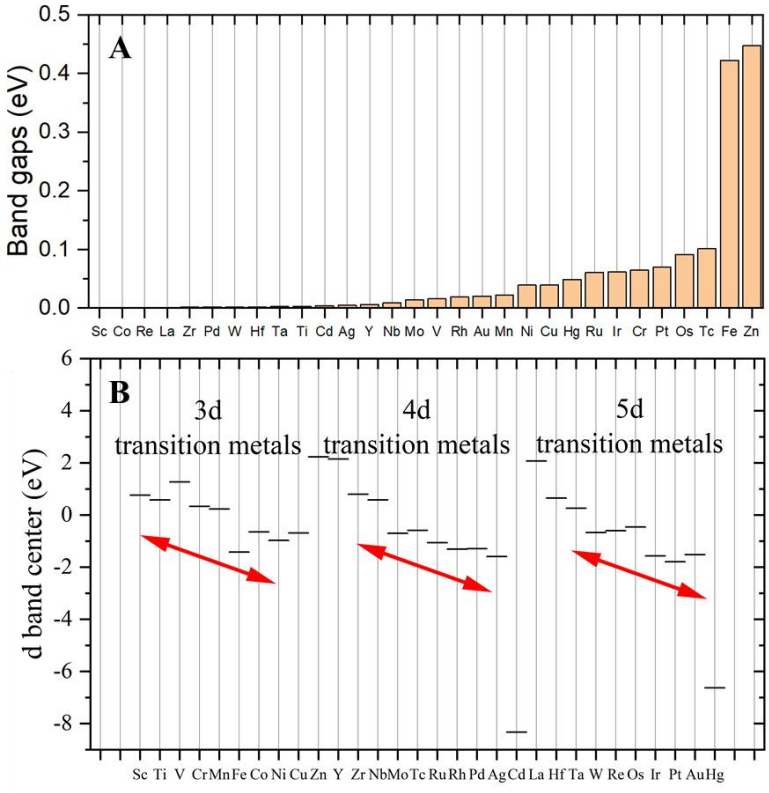
105

106 **3. Screening for lower band gaps and higher electronic conductivity**

107 **Supplementary Table 18. Valence band maximums (VBMs), conduction band**
108 **minimums (CBMs), fermi levels, and band gaps of $LiFePO_4$ before and after**
109 **doping by 3d, 4d and 5d transition metals.**

Materials	VBM (eV)	CBM (eV)	Fermi level (eV)	Band gaps (eV)
Sc-$LiFePO_4$	5.75	5.75	5.75	0.00
Ti-$LiFePO_4$	5.62	5.62	5.62	0.00
V-$LiFePO_4$	5.22	5.23	5.23	0.01
Cr-$LiFePO_4$	5.21	5.28	5.24	0.06
Mn-$LiFePO_4$	4.94	4.97	4.95	0.02
$LiFePO_4$	4.72	5.14	4.95	0.42
Co-$LiFePO_4$	4.64	4.64	4.64	0.00
Ni-$LiFePO_4$	4.46	4.50	4.49	0.03
Cu-$LiFePO_4$	4.33	4.37	4.34	0.03
Zn-$LiFePO_4$	4.70	5.14	4.93	0.44
Y-$LiFePO_4$	5.59	5.59	5.59	0.01
Zr-$LiFePO_4$	5.70	5.70	5.70	0.00
Nb-$LiFePO_4$	5.21	5.22	5.22	0.01
Mo-$LiFePO_4$	5.69	5.71	5.70	0.01
Tc-$LiFePO_4$	5.23	5.33	5.28	0.10
Ru-$LiFePO_4$	5.26	5.31	5.31	0.06
Rh-$LiFePO_4$	4.76	4.78	4.78	0.02
Pd-$LiFePO_4$	4.18	4.18	4.18	0.00
Ag-$LiFePO_4$	3.65	3.65	3.65	0.00
Cd-$LiFePO_4$	4.67	4.67	4.67	0.00
La-$LiFePO_4$	6.02	6.02	6.02	0.00
Hf-$LiFePO_4$	5.97	5.97	5.97	0.00
Ta-$LiFePO_4$	5.46	5.46	5.46	0.00
W-$LiFePO_4$	5.76	5.76	5.76	0.00
Re-$LiFePO_4$	5.62	5.62	5.62	0.00
Os-$LiFePO_4$	5.32	5.42	5.35	0.09
Ir-$LiFePO_4$	5.26	5.32	5.27	0.06
Pt-$LiFePO_4$	4.52	4.59	4.54	0.07
Au-$LiFePO_4$	3.51	3.75	3.73	0.02
Hg-$LiFePO_4$	4.52	4.57	4.54	0.05

110



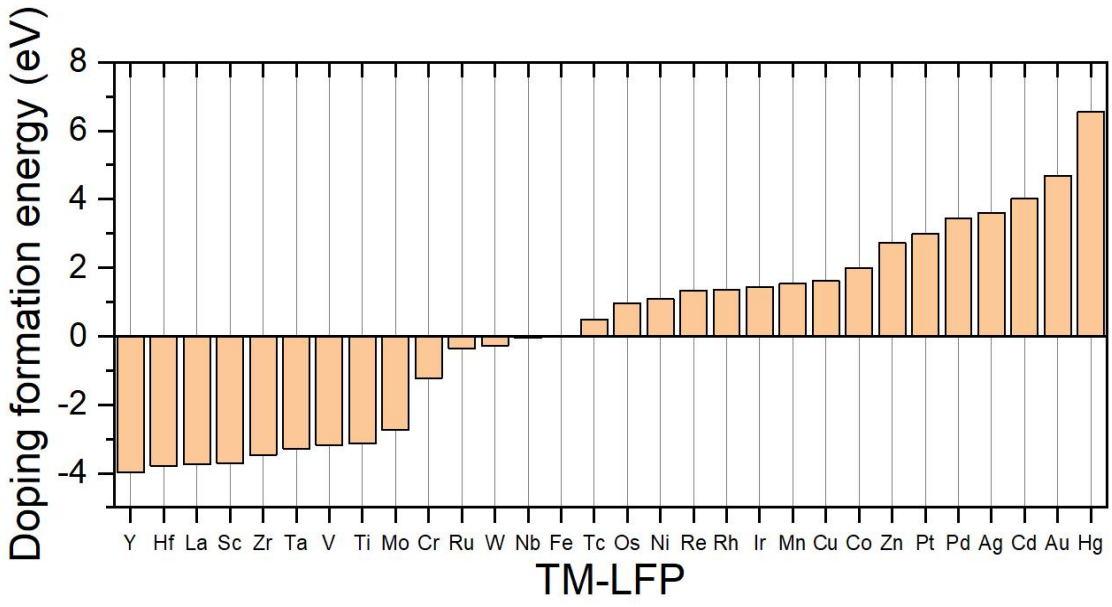
Supplementary Figure 9. Band gaps and d band centers of TM-LFP models.

115 **4. Screening for easier to be fromed**

116 **Supplementary Table 19. Cell energy and formation energy of the TM doped LFP**
117 **models. (The cell energy of LFP is -196.28 eV and the chemical potential of Fe is**
118 **-3.40 eV)**

Materials	Cell energy (eV)	Chemical potential of TM (eV)	Formation energy (eV)
Sc-$LiFePO_4$	-198.72	-2.14	-3.70
Ti-$LiFePO_4$	-198.27	-2.25	-3.14
V-$LiFePO_4$	-198.22	-2.16	-3.18
Cr-$LiFePO_4$	-198.20	-4.10	-1.22
Mn-$LiFePO_4$	-196.49	-5.16	1.55
$LiFePO_4$	-196.28	-3.40	0.00
Co-$LiFePO_4$	-192.72	-1.83	2.00
Ni-$LiFePO_4$	-192.54	-0.74	1.08
Cu-$LiFePO_4$	-191.51	-0.24	1.61
Zn-$LiFePO_4$	-190.32	-0.17	2.73
Y-$LiFePO_4$	-199.18	-2.33	-3.97
Zr-$LiFePO_4$	-198.67	-2.32	-3.47
Nb-$LiFePO_4$	-196.07	-3.14	-0.05
Mo-$LiFePO_4$	-196.93	-1.31	-2.74
Tc-$LiFePO_4$	-195.67	-3.28	0.49
Ru-$LiFePO_4$	-194.54	-1.31	-0.35
Rh-$LiFePO_4$	-192.82	-1.29	1.35
Pd-$LiFePO_4$	-190.92	-1.48	3.43
Ag-$LiFePO_4$	-189.62	-0.34	3.60
Cd-$LiFePO_4$	-189.03	-0.17	4.02
La-$LiFePO_4$	-197.34	-0.73	-3.74
Hf-$LiFePO_4$	-200.22	-3.55	-3.79
Ta-$LiFePO_4$	-199.63	-3.47	-3.28
W-$LiFePO_4$	-197.70	-4.54	-0.28
Re-$LiFePO_4$	-196.15	-4.61	1.34
Os-$LiFePO_4$	-194.82	-2.91	0.97
Ir-$LiFePO_4$	-192.71	-1.27	1.44
Pt-$LiFePO_4$	-190.43	-0.53	2.98
Au-$LiFePO_4$	-188.48	-0.29	4.69
Hg-$LiFePO_4$	-186.45	-0.12	6.55

119



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121 **Supplementary Figure 10. Doping formation energy of TM-LFP models.**

122

5. Screening for higher elastic properties

Supplementary Table 20. Stiffness coefficients of Sc-LFP.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1580.6044	515.6936	425.8139	72.1389	-4.7406	-3.5705
YY	515.6936	1245.0663	641.5577	32.3296	24.5931	3.9971
ZZ	425.8139	641.5577	1698.3755	-46.6619	-2.1627	-1.3015
XY	72.1389	32.3296	-46.6619	382.1998	-4.1809	-0.0775
YZ	-4.7406	24.5931	-2.1627	-4.1809	342.4068	3.712
ZX	-3.5705	3.9971	-1.3015	-0.0775	3.712	308.3293

Supplementary Table 21. Stiffness coefficients of Ti-LFP.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1596.2384	539.2559	425.0723	14.5701	-0.5414	20.8603
YY	539.2559	1296.5331	697.2491	-15.3149	-3.8194	4.7936
ZZ	425.0723	697.2491	1827.9295	-61.6606	3.8782	26.4244
XY	14.5701	-15.3149	-61.6606	442.6915	-6.2147	-1.6695
YZ	-0.5414	-3.8194	3.8782	-6.2147	367.6011	-8.6403
ZX	20.8603	4.7936	26.4244	-1.6695	-8.6403	356.1393

Supplementary Table 22. Stiffness coefficients of V-LFP.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1304.4988	405.6993	510.2391	307.9182	1.9661	8.8618
YY	405.6993	1271.9255	696.2905	183.1896	-15.1927	20.6615
ZZ	510.2391	696.2905	2244.5405	153.1432	0.4925	13.1892
XY	307.9182	183.1896	153.1432	462.5294	5.2854	-2.2861
YZ	1.9661	-15.1927	0.4925	5.2854	425.3541	-10.7092
ZX	8.8618	20.6615	13.1892	-2.2861	-10.7092	387.1381

Supplementary Table 23. Stiffness coefficients of Cr-LFP.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1704.8205	773.5011	822.1143	1.3602	12.0019	8.559
YY	773.5011	1319.1751	737.2364	107.6628	16.3508	-35.7566
ZZ	822.1143	737.2364	2249.2206	24.5773	-30.1759	-4.8494
XY	1.3602	107.6628	24.5773	437.6912	-0.2112	23.7661
YZ	12.0019	16.3508	-30.1759	-0.2112	82.6878	95.6989
ZX	8.559	-35.7566	-4.8494	23.7661	95.6989	352.6975

Supplementary Table 24. Stiffness coefficients of Mn-LFP.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1695.015	520.1184	442.8975	22.2799	-1.8958	-4.2538
YY	520.1184	1234.0151	611.3278	49.4195	-0.9147	-1.688
ZZ	442.8975	611.3278	1575.5522	-30.801	-5.9754	21.0453
XY	22.2799	49.4195	-30.801	331.1076	0.2313	1.2342
YZ	-1.8958	-0.9147	-5.9754	0.2313	393.2787	-7.6147
ZX	-4.2538	-1.688	21.0453	1.2342	-7.6147	374.2086

Supplementary Table 25. Stiffness coefficients of LFP.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1730.9278	568.7318	484.0128	-5.2054	1.2992	-1.9373
YY	568.7318	1369.2525	688.9731	-11.8125	0.0699	-2.1925
ZZ	484.0128	688.9731	1938.8482	1.2619	0.7919	-0.6945
XY	-5.2054	-11.8125	1.2619	463.8531	0.4068	-0.2767
YZ	1.2992	0.0699	0.7919	0.4068	390.582	-0.1823
ZX	-1.9373	-2.1925	-0.6945	-0.2767	-0.1823	389.4142

Supplementary Table 26. Stiffness coefficients of Co-LFP.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	575.4631	-1381.5437	306.9014	-87.9808	-4.1791	1.5458
YY	-1381.5437	-435.8431	135.9981	32.6102	-5.8534	-263.7345
ZZ	306.9014	135.9981	2544.6894	18.5588	9.1474	-289.5848
XY	-87.9808	32.6102	18.5588	452.742	-6.741	-13.9651
YZ	-4.1791	-5.8534	9.1474	-6.741	420.113	-5.371
ZX	1.5458	-263.7345	-289.5848	-13.9651	-5.371	360.8728

Supplementary Table 27. Stiffness coefficients of Ni-LFP.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1853.7521	598.4548	512.7407	19.0662	-14.5689	0.8172
YY	598.4548	1396.4859	672.3862	37.6373	-7.6493	-0.1681
ZZ	512.7407	672.3862	1818.0979	35.8854	-5.2766	1.7588
XY	19.0662	37.6373	35.8854	467.3682	0.6063	0.2833
YZ	-14.5689	-7.6493	-5.2766	0.6063	418.9794	12.5597
ZX	0.8172	-0.1681	1.7588	0.2833	12.5597	402.236

Supplementary Table 28. Stiffness coefficients of Cu-LFP.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1387.107	207.4941	75.2574	70.6131	-41.5637	-68.0912
YY	207.4941	1056.2167	344.0044	72.9834	-40.94	-63.6251
ZZ	75.2574	344.0044	1394.768	110.1726	-41.708	-65.8296
XY	70.6131	72.9834	110.1726	401.1328	5.1603	-2.919
YZ	-41.5637	-40.94	-41.708	5.1603	366.321	62.2478
ZX	-68.0912	-63.6251	-65.8296	-2.919	62.2478	333.1236

Supplementary Table 29. Stiffness coefficients of Zn-LFP.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1741.0012	543.0981	458.7521	7.4685	-0.4775	-6.8885
YY	543.0981	1401.2155	685.989	-26.2984	-2.2774	-7.2002
ZZ	458.7521	685.989	1874.0799	33.8848	-0.3429	-5.3679
XY	7.4685	-26.2984	33.8848	475.3757	-0.0202	0.3349
YZ	-0.4775	-2.2774	-0.3429	-0.0202	347.965	56.5184
ZX	-6.8885	-7.2002	-5.3679	0.3349	56.5184	356.0804

Supplementary Table 30. Stiffness coefficients of Y-LFP.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1440.8779	490.5088	409.0916	40.0319	10.8259	-0.6809
YY	490.5088	1127.2385	607.343	85.9679	3.2625	-11.2896
ZZ	409.0916	607.343	1470.1224	-93.0685	7.2275	-5.4394
XY	40.0319	85.9679	-93.0685	328.8804	2.9299	2.7171
YZ	10.8259	3.2625	7.2275	2.9299	304.3877	-44.0788
ZX	-0.6809	-11.2896	-5.4394	2.7171	-44.0788	230.8204

Supplementary Table 31. Stiffness coefficients of Zr-LFP.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1460.8419	487.0736	339.0046	57.8079	1.8569	2.9118
YY	487.0736	1204.7312	616.0132	81.3087	1.9191	1.1396
ZZ	339.0046	616.0132	1563.5388	-73.193	10.4245	-1.0962
XY	57.8079	81.3087	-73.193	359.0014	0.5508	3.0229
YZ	1.8569	1.9191	10.4245	0.5508	297.1034	-14.005
ZX	2.9118	1.1396	-1.0962	3.0229	-14.005	276.8611

Supplementary Table 32. Stiffness coefficients of Nb-LFP.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1565.14	578.5849	443.3643	-5.2461	14.7177	-5.6458
YY	578.5849	1244.3958	677.7651	19.2306	3.5036	1.4299
ZZ	443.3643	677.7651	1704.7556	-106.8052	9.0407	-4.3448
XY	-5.2461	19.2306	-106.8052	407.8805	-2.0626	6.4607
YZ	14.7177	3.5036	9.0407	-2.0626	339.4987	-59.9209
ZX	-5.6458	1.4299	-4.3448	6.4607	-59.9209	335.8174

Supplementary Table 33. Stiffness coefficients of Mo-LFP.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	2045.4757	792.5815	678.3007	17.5222	23.7647	-0.5677
YY	792.5815	1306.9002	656.9263	36.3463	9.1937	-13.8225
ZZ	678.3007	656.9263	1681.3341	-41.8608	-9.1497	-16.849
XY	17.5222	36.3463	-41.8608	413.4298	10.8053	11.4789
YZ	23.7647	9.1937	-9.1497	10.8053	340.2529	-13.4457
ZX	-0.5677	-13.8225	-16.849	11.4789	-13.4457	337.3261

Supplementary Table 34. Stiffness coefficients of Tc-LFP.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	-13579.414	-14288.9115	-13375.1412	-1123.9551	24.8521	-2.8516
YY	-14288.9115	-14813.892	-14683.9231	-1721.7402	-61.5404	-42.79
ZZ	-13375.1412	-14683.9231	-13066.38	-1882.8707	-94.4987	-33.3129
XY	-1123.9551	-1721.7402	-1882.8707	142.4781	-36.1249	-19.6335
YZ	24.8521	-61.5404	-94.4987	-36.1249	405.1698	-55.4901
ZX	-2.8516	-42.79	-33.3129	-19.6335	-55.4901	389.3217

Supplementary Table 35. Stiffness coefficients of Ru-LFP.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1777.2798	623.7477	534.4032	-144.7946	-0.8382	3.572
YY	623.7477	1391.9799	698.6787	-158.8269	7.5991	1.1108
ZZ	534.4032	698.6787	1925.7202	-174.7383	4.5601	4.594
XY	-144.7946	-158.8269	-174.7383	607.4577	9.7864	15.1354
YZ	-0.8382	7.5991	4.5601	9.7864	450.4275	-49.0787
ZX	3.572	1.1108	4.594	15.1354	-49.0787	435.2067

Supplementary Table 36. Stiffness coefficients of Rh-LFP.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1696.013	469.9906	504.415	-13.2494	1.6075	-2.6999
YY	469.9906	1254.098	595.0138	-17.1641	-5.7615	-13.2913
ZZ	504.415	595.0138	1783.1312	-12.7009	-1.3093	-4.513
XY	-13.2494	-17.1641	-12.7009	454.0191	1.2642	1.2319
YZ	1.6075	-5.7615	-1.3093	1.2642	378.2164	-1.6177
ZX	-2.6999	-13.2913	-4.513	1.2319	-1.6177	394.4124

Supplementary Table 37. Stiffness coefficients of Pd-LFP.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1546.1732	104.892	363.7558	22.342	9.1144	-26.4054
YY	104.892	895.2986	248.9451	85.6085	21.1964	14.9065
ZZ	363.7558	248.9451	1619.2776	1.3208	11.395	-27.3006
XY	22.342	85.6085	1.3208	377.1686	-2.4937	4.2864
YZ	9.1144	21.1964	11.395	-2.4937	363.9939	-13.875
ZX	-26.4054	14.9065	-27.3006	4.2864	-13.875	362.5201

Supplementary Table 38. Stiffness coefficients of Ag-LFP.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1480.0951	204.1278	522.9476	-40.999	-1.4823	14.1556
YY	204.1278	1388.6966	505.7613	91.8476	-34.0655	4.587
ZZ	522.9476	505.7613	1680.2461	-128.1445	-9.132	3.5063
XY	-40.999	91.8476	-128.1445	311.2045	1.6298	-2.4636
YZ	-1.4823	-34.0655	-9.132	1.6298	341.1914	-7.4718
ZX	14.1556	4.587	3.5063	-2.4636	-7.4718	313.298

Supplementary Table 39. Stiffness coefficients of Cd-LFP.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1614.5087	506.8332	483.4431	245.0648	0.0325	-5.0635
YY	506.8332	1245.2721	705.0958	103.3785	-7.5414	-18.6835
ZZ	483.4431	705.0958	1771.3306	203.6592	8.217	-3.2378
XY	245.0648	103.3785	203.6592	403.026	2.4745	10.6146
YZ	0.0325	-7.5414	8.217	2.4745	369.6494	-37.79
ZX	-5.0635	-18.6835	-3.2378	10.6146	-37.79	348.7228

147 **Supplementary Table 40. Stiffness coefficients of La-LFP.**

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	385.2822	398.7219	-68.6547	-30.0129	-11.4126	31.1593
YY	398.7219	1069.4984	620.5863	162.6799	-0.1466	5.8922
ZZ	-68.6547	620.5863	1168.5157	-110.1589	6.1699	12.7881
XY	-30.0129	162.6799	-110.1589	225.4915	-5.2865	-2.5888
YZ	-11.4126	-0.1466	6.1699	-5.2865	262.526	-45.4913
ZX	31.1593	5.8922	12.7881	-2.5888	-45.4913	187.5298

148 **Supplementary Table 41. Stiffness coefficients of Hf-LFP.**

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1313.8743	499.7524	325.5809	82.3254	1.7762	-26.4904
YY	499.7524	1114.8283	617.5033	81.8669	0.9248	-28.1802
ZZ	325.5809	617.5033	1607.6499	-32.3079	4.3524	-25.3356
XY	82.3254	81.8669	-32.3079	327.2503	-3.0456	8.0738
YZ	1.7762	0.9248	4.3524	-3.0456	261.01	-4.5856
ZX	-26.4904	-28.1802	-25.3356	8.0738	-4.5856	249.9034

149 **Supplementary Table 42. Stiffness coefficients of Ta-LFP.**

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	2015.0507	955.6891	668.4839	35.0651	-16.0563	-25.5722
YY	955.6891	1842.0802	1287.9589	4.8778	3.3749	-0.7779
ZZ	668.4839	1287.9589	1798.9898	0.2258	-102.9149	-23.7197
XY	35.0651	4.8778	0.2258	412.4522	-11.8514	22.0475
YZ	-16.0563	3.3749	-102.9149	-11.8514	436.7409	-46.3916
ZX	-25.5722	-0.7779	-23.7197	22.0475	-46.3916	310.6983

150 **Supplementary Table 43. Stiffness coefficients of W-LFP.**

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1556.6416	685.7409	298.938	64.7085	-5.5908	5.3914
YY	685.7409	1379.4471	654.3254	21.9551	-26.3185	1.4359
ZZ	298.938	654.3254	1363.7419	-27.7674	-12.9379	4.1655
XY	64.7085	21.9551	-27.7674	441.7617	-8.1393	1.1211
YZ	-5.5908	-26.3185	-12.9379	-8.1393	346.4766	-11.1176
ZX	5.3914	1.4359	4.1655	1.1211	-11.1176	320.9381

151 **Supplementary Table 44. Stiffness coefficients of Re-LFP.**

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1361.9809	542.7183	296.3951	-266.9267	15.1813	20.7456
YY	542.7183	1357.93	657.7856	-186.5075	28.4149	25.8746
ZZ	296.3951	657.7856	1737.9632	-363.9815	10.9969	12.0649
XY	-266.9267	-186.5075	-363.9815	254.9487	36.1643	107.7715
YZ	15.1813	28.4149	10.9969	36.1643	380.6593	-53.4953
ZX	20.7456	25.8746	12.0649	107.7715	-53.4953	362.7787

152

Supplementary Table 45. Stiffness coefficients of Os-LFP.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	2183.5805	1396.8077	954.6677	5.9512	-23.0423	-5.5383
YY	1396.8077	1919.5352	1158.4064	83.6328	-2.8798	-10.0691
ZZ	954.6677	1158.4064	2288.3065	-60.1683	18.4238	-26.3859
XY	5.9512	83.6328	-60.1683	507.9037	0.7648	2.0319
YZ	-23.0423	-2.8798	18.4238	0.7648	419.7906	-63.3823
ZX	-5.5383	-10.0691	-26.3859	2.0319	-63.3823	409.7143

Supplementary Table 46. Stiffness coefficients of Ir-LFP.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1685.9112	912.4245	504.0928	40.4834	6.384	0.3732
YY	912.4245	1991.4551	880.414	96.2326	21.5268	-1.0876
ZZ	504.0928	880.414	1700.4394	7.4137	1.5985	-1.6162
XY	40.4834	96.2326	7.4137	471.3755	0.1441	0.672
YZ	6.384	21.5268	1.5985	0.1441	350.4964	21.2724
ZX	0.3732	-1.0876	-1.6162	0.672	21.2724	352.6974

Supplementary Table 47. Stiffness coefficients of Pt-LFP.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1586.4989	303.3234	538.1281	1176.139	0.7929	-2.2379
YY	303.3234	562.9906	458.4948	818.5974	-10.1747	-39.3323
ZZ	538.1281	458.4948	1692.5645	1023.815	-7.9011	4.2258
XY	1176.139	818.5974	1023.815	191.2825	-12.7519	-34.7136
YZ	0.7929	-10.1747	-7.9011	-12.7519	354.0229	-10.0343
ZX	-2.2379	-39.3323	4.2258	-34.7136	-10.0343	328.491

Supplementary Table 48. Stiffness coefficients of Au-LFP.

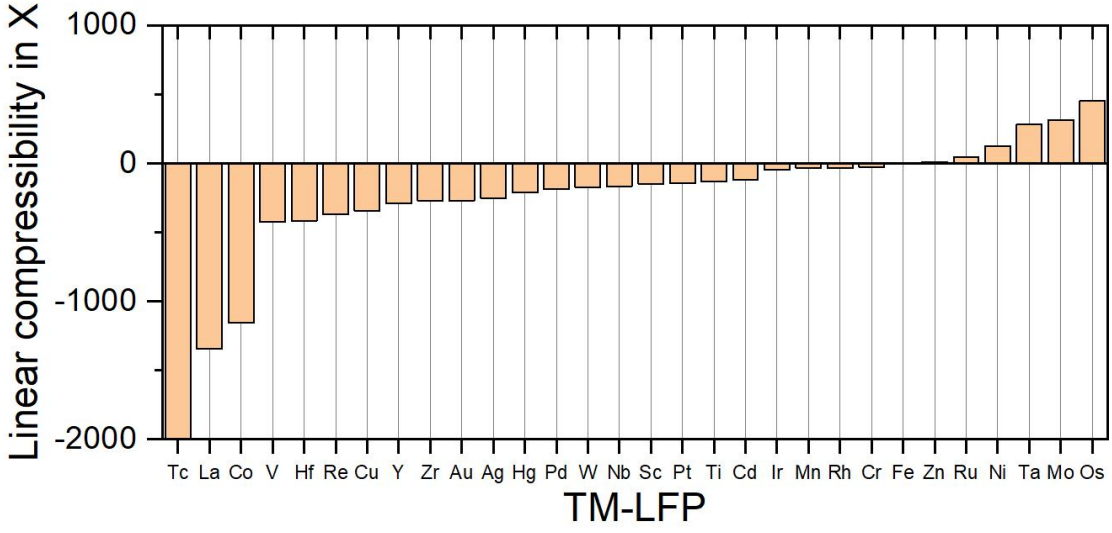
Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1461.2413	420.5353	420.745	-141.3761	-9.5636	1.0417
YY	420.5353	1018.1808	625.6254	75.6162	-4.6666	-7.3733
ZZ	420.745	625.6254	1685.6116	-106.0843	10.9899	8.9334
XY	-141.3761	75.6162	-106.0843	184.2949	1.7759	-0.9082
YZ	-9.5636	-4.6666	10.9899	1.7759	205.982	40.5733
ZX	1.0417	-7.3733	8.9334	-0.9082	40.5733	254.2851

Supplementary Table 49. Stiffness coefficients of Hg-LFP.

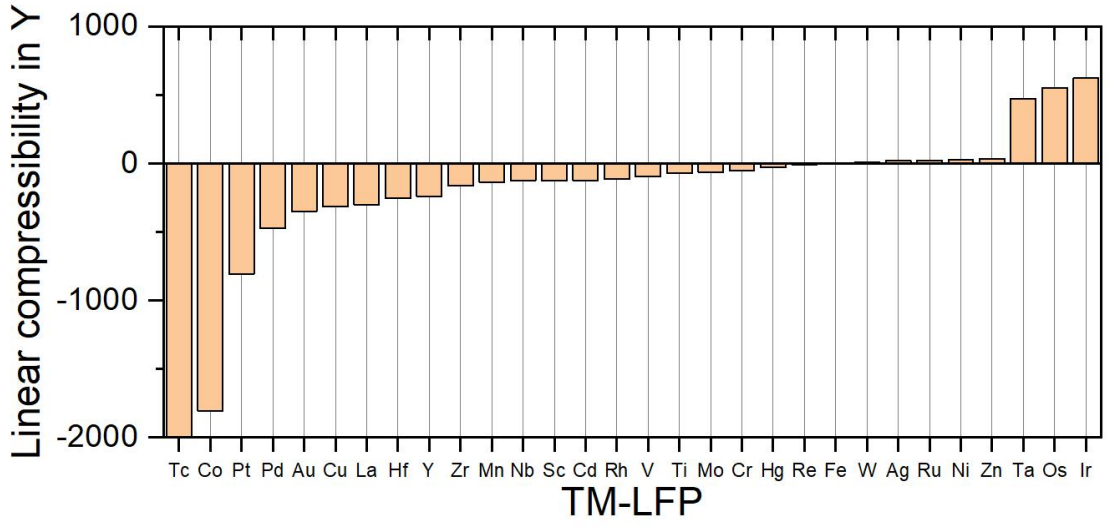
Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1518.3575	479.4202	513.9325	-51.2488	-3.0769	-11.7599
YY	479.4202	1338.9202	617.4294	87.0834	-16.729	-37.1504
ZZ	513.9325	617.4294	1359.4245	-69.4272	-28.4516	-103.1327
XY	-51.2488	87.0834	-69.4272	325.8795	-4.139	-4.6519
YZ	-3.0769	-16.729	-28.4516	-4.139	267.876	-34.6459
ZX	-11.7599	-37.1504	-103.1327	-4.6519	-34.6459	266.1079

Supplementary Table 50. Summary of stiffness coefficients (difference of TM-LFP with LFP).

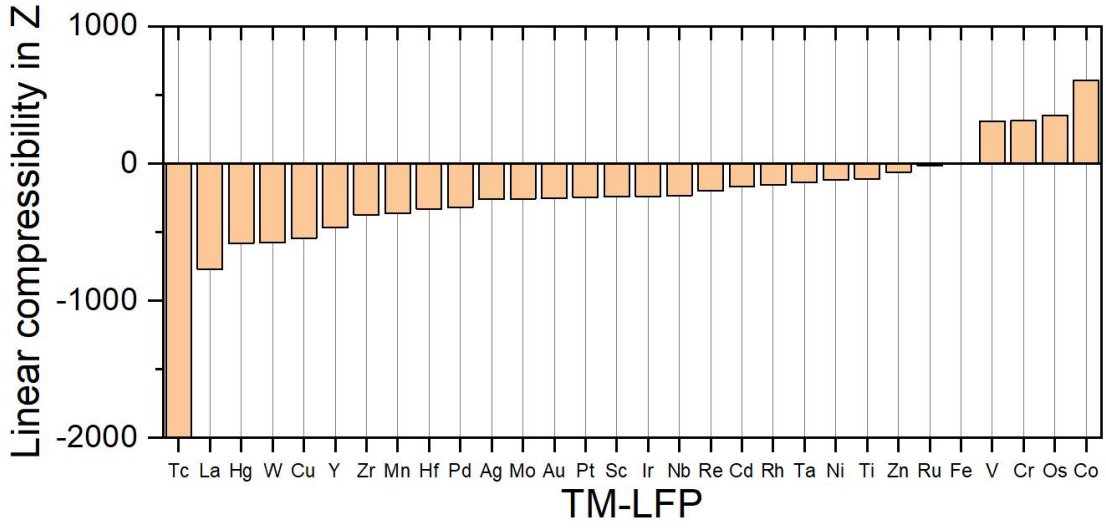
No.	TM	X	Y	Z	XY	YZ	ZX
1	Sc	-150.323	-124.186	-240.473	-81.6533	-48.1752	-81.0849
2	Ti	-134.689	-72.7194	-110.919	-21.1616	-22.9809	-33.2749
3	V	-426.429	-97.327	305.6923	-1.3237	34.7721	-2.2761
4	Cr	-26.1073	-50.0774	310.3724	-26.1619	-307.894	-36.7167
5	Mn	-35.9128	-135.237	-363.296	-132.746	2.6967	-15.2056
6	Fe	0	0	0	0	0	0
7	Co	-1155.46	-1805.1	605.8412	-11.1111	29.531	-28.5414
8	Ni	122.8243	27.2334	-120.75	3.5151	28.3974	12.8218
9	Cu	-343.821	-313.036	-544.08	-62.7203	-24.261	-56.2906
10	Zn	10.0734	31.963	-64.7683	11.5226	-42.617	-33.3338
11	Y	-290.05	-242.014	-468.726	-134.973	-86.1943	-158.594
12	Zr	-270.086	-164.521	-375.309	-104.852	-93.4786	-112.553
13	Nb	-165.788	-124.857	-234.093	-55.9726	-51.0833	-53.5968
14	Mo	314.5479	-62.3523	-257.514	-50.4233	-50.3291	-52.0881
15	Tc	-15310.3	-16183.1	-15005.2	-321.375	14.5878	-0.0925
16	Ru	46.352	22.7274	-13.128	143.6046	59.8455	45.7925
17	Rh	-34.9148	-115.155	-155.717	-9.834	-12.3656	4.9982
18	Pd	-184.755	-473.954	-319.571	-86.6845	-26.5881	-26.8941
19	Ag	-250.833	19.4441	-258.602	-152.649	-49.3906	-76.1162
20	Cd	-116.419	-123.98	-167.518	-60.8271	-20.9326	-40.6914
21	La	-1345.65	-299.754	-770.333	-238.362	-128.056	-201.884
22	Hf	-417.054	-254.424	-331.198	-136.603	-129.572	-139.511
23	Ta	284.1229	472.8277	-139.858	-51.4009	46.1589	-78.7159
24	W	-174.286	10.1946	-575.106	-22.0914	-44.1054	-68.4761
25	Re	-368.947	-11.3225	-200.885	-208.904	-9.9227	-26.6355
26	Os	452.6527	550.2827	349.4583	44.0506	29.2086	20.3001
27	Ir	-45.0166	622.2026	-238.409	7.5224	-40.0856	-36.7168
28	Pt	-144.429	-806.262	-246.284	-272.571	-36.5591	-60.9232
29	Au	-269.687	-351.072	-253.237	-279.558	-184.6	-135.129
30	Hg	-212.57	-30.3323	-579.424	-137.974	-122.706	-123.306



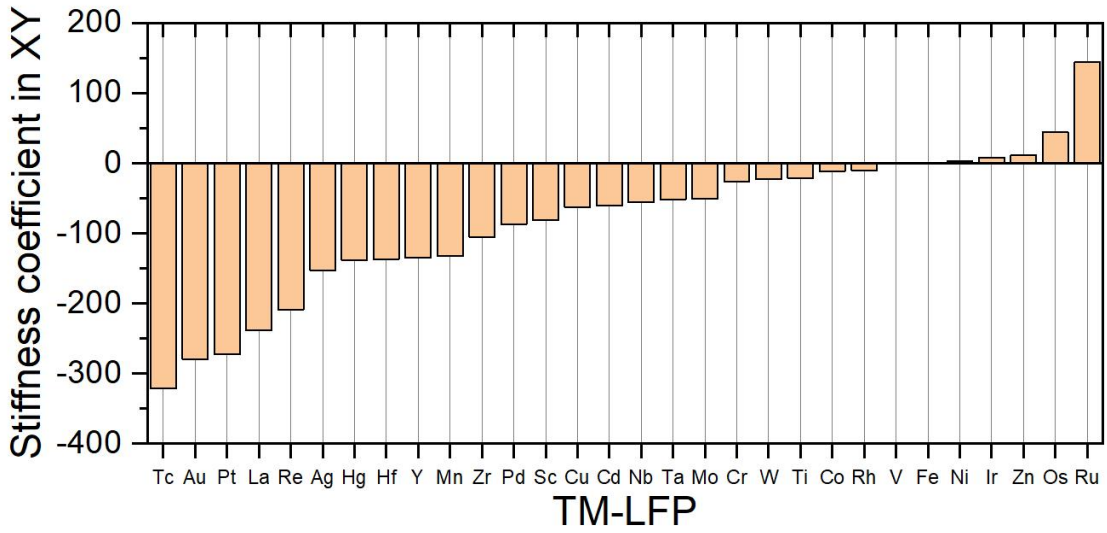
Supplementary Figure 11. Summary of stiffness coefficients (difference of TM-LFP with LFP) in X.



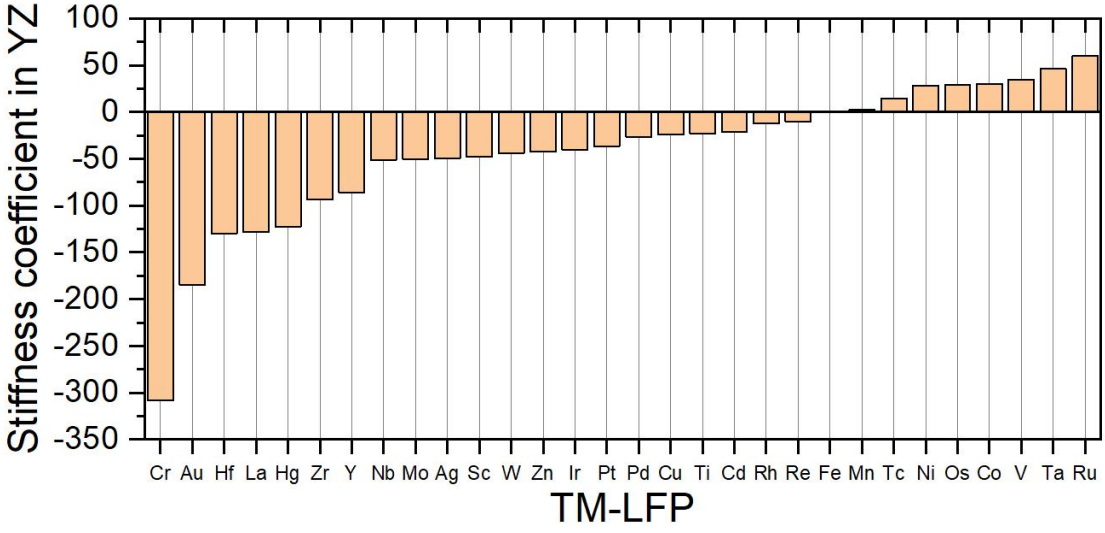
Supplementary Figure 12. Summary of stiffness coefficients (difference of TM-LFP with LFP) in Y.



Supplementary Figure 13. Summary of stiffness coefficients (difference of TM-LFP with LFP) in Z.



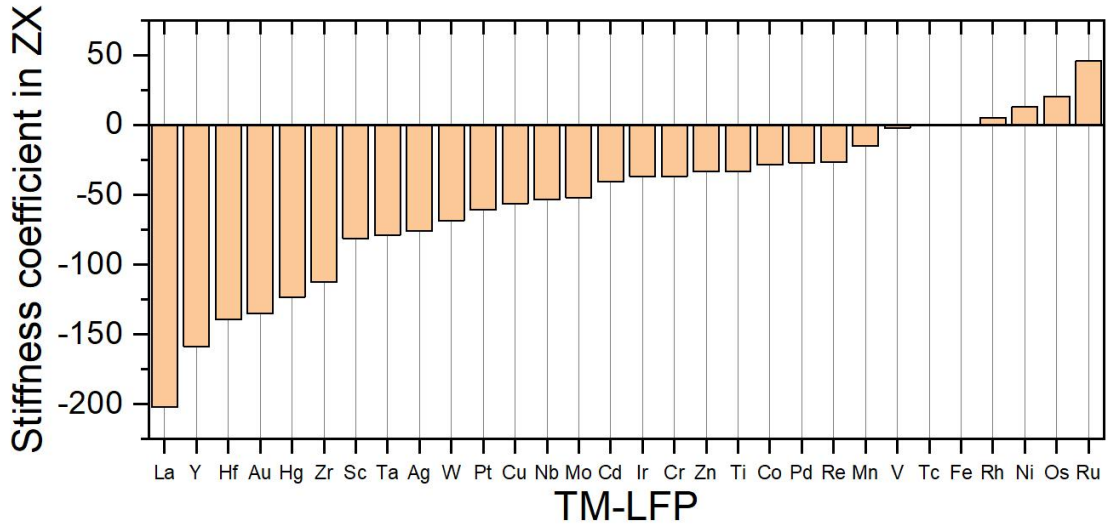
Supplementary Figure 14. Stiffness coefficients (difference of TM-LFP with LFP) in XY.



176

177 **Supplementary Figure 15. Stiffness coefficients (difference of TM-LFP with LFP)**

178 **in YZ.**



179

180 **Supplementary Figure 16. Stiffness coefficients (difference of TM-LFP with LFP)**

181 **in ZX.**

182

Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
		Z	Z			Z	X,Y		X,Y
Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd
			X		X,Y			Y	
La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg
		X,Y	Y		X,Y,Z	Y			

183

184 **Supplementary Figure 17. Summary of linear compressibility of TM-LFP models.**
185 **The yellow area indicates the models with higher linear compressibility than pure**
186 **LFP. The X, Y and Z indicate the directions of a particular TM-LFP models.**

Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
		YZ		YZ		YZ	XY,YZ,ZX		XY
Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd
					XY,YZ,ZX	ZX			
La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg
		YZ			XY,YZ,ZX	XY			

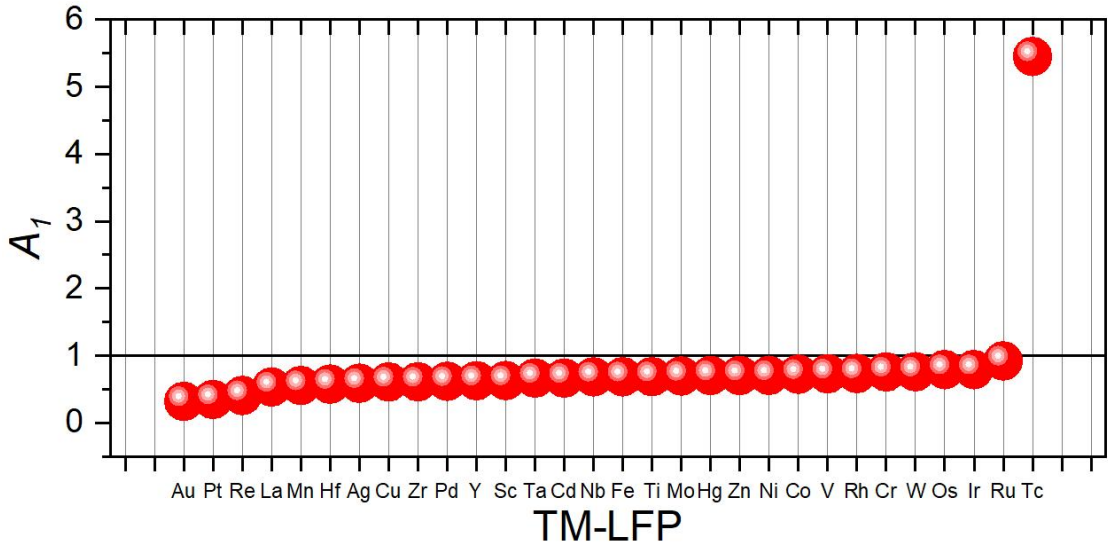
187

188 **Supplementary Figure 18. Summary of shear strength of TM-LFP models. The**
189 **green area indicates the models with higher shear strength than pure LFP. The**
190 **XY, YZ and ZX indicate the directions of a particular TM-LFP models.**
191

6. Screening for higher isotropy

Supplementary Table 51. Anisotropy shear moduluses (A_i) of all the TM-LFP models.

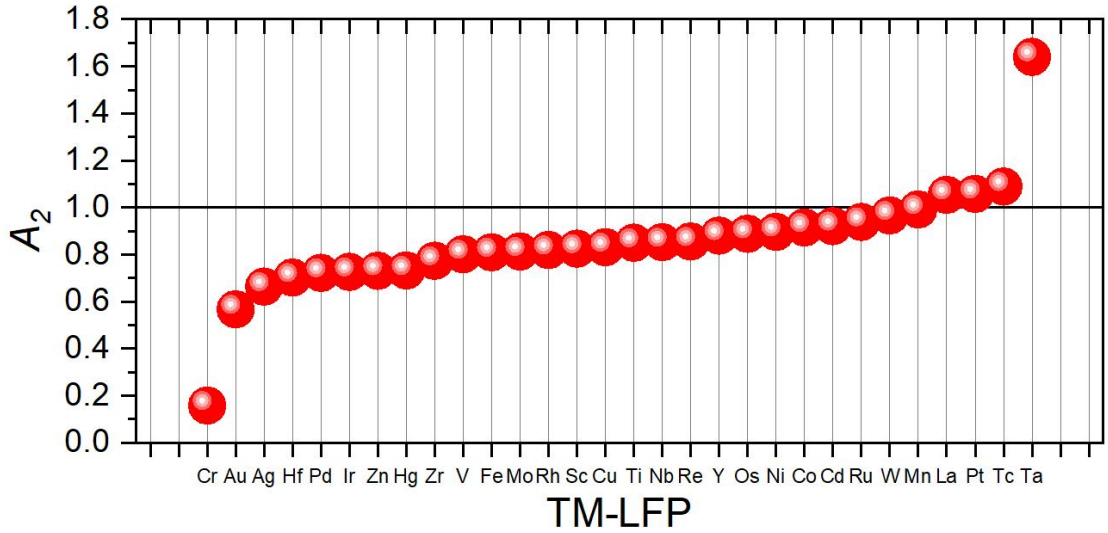
Materials	A_1	A_2	A_3
Sc-$LiFePO_4$	0.629821772	0.824914426	0.68735916
Ti-$LiFePO_4$	0.687937	0.849962	0.7852
V-$LiFePO_4$	0.731687915	0.801086876	0.877354024
Cr-$LiFePO_4$	0.757968363	0.157957678	0.955176915
Mn-$LiFePO_4$	0.555369775	0.991305817	0.792481845
$LiFePO_4$	0.686745	0.809432	0.793623
Co-$LiFePO_4$	0.722552005	0.914855273	0.497291322
Ni-$LiFePO_4$	0.706429482	0.896303018	0.783578506
Cu-$LiFePO_4$	0.609772543	0.831142388	0.656939841
Zn-$LiFePO_4$	0.704892899	0.731281078	0.692756517
Y-$LiFePO_4$	0.628588901	0.880576338	0.581741729
Zr-$LiFePO_4$	0.612011184	0.773584085	0.654740122
Nb-$LiFePO_4$	0.684602464	0.852144035	0.812937085
Mo-$LiFePO_4$	0.69771	0.812844	0.763521
Tc-$LiFePO_4$	5.454312632	1.08947789	8.439801211
Ru-$LiFePO_4$	0.922419	0.938223	0.905848
Rh-$LiFePO_4$	0.735160086	0.819004055	0.784849615
Pd-$LiFePO_4$	0.61883184	0.721964451	0.649768485
Ag-$LiFePO_4$	0.588720639	0.663338324	0.509316649
Cd-$LiFePO_4$	0.666446985	0.920435373	0.755582211
La-$LiFePO_4$	0.533358232	1.053431263	1.141148951
Hf-$LiFePO_4$	0.57656	0.701889	0.699423
Ta-$LiFePO_4$	0.666031643	1.640107019	0.638721046
W-$LiFePO_4$	0.760836	0.966099	0.820495
Re-$LiFePO_4$	0.406753969	0.855259442	0.887817447
Os-$LiFePO_4$	0.792809323	0.887962315	1.251513421
Ir-$LiFePO_4$	0.792839017	0.72601622	0.761552726
Pt-$LiFePO_4$	0.347343154	1.0579173	0.851651306
Au-$LiFePO_4$	0.31976727	0.567231947	0.62083161
Hg-$LiFePO_4$	0.704635938	0.732158745	0.560688309



196

197 **Supplementary Figure 19. Anisotropy shear moduluses of the <010> and <011>**

198 **directions of {100} planes.**

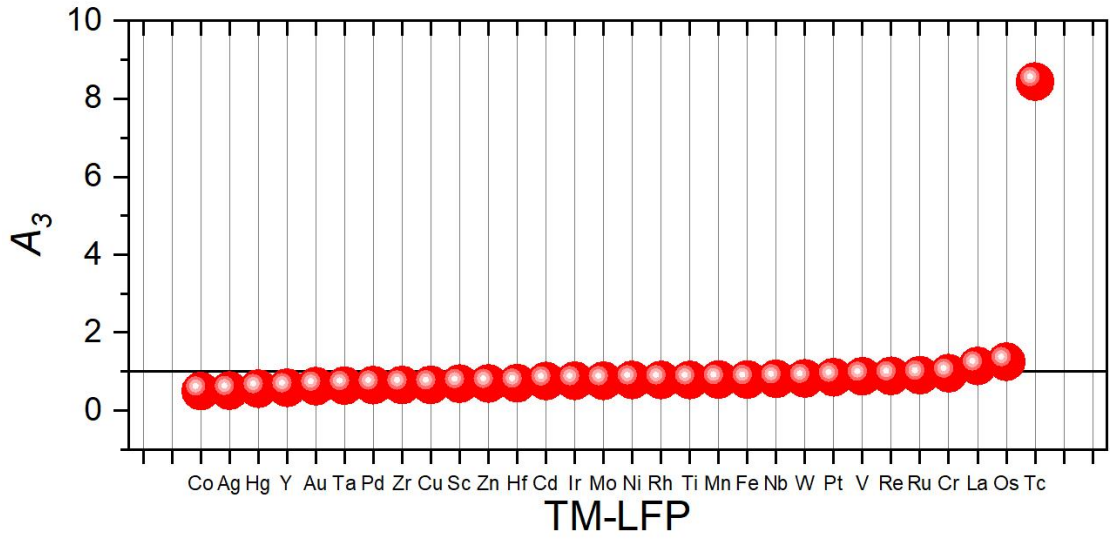


199

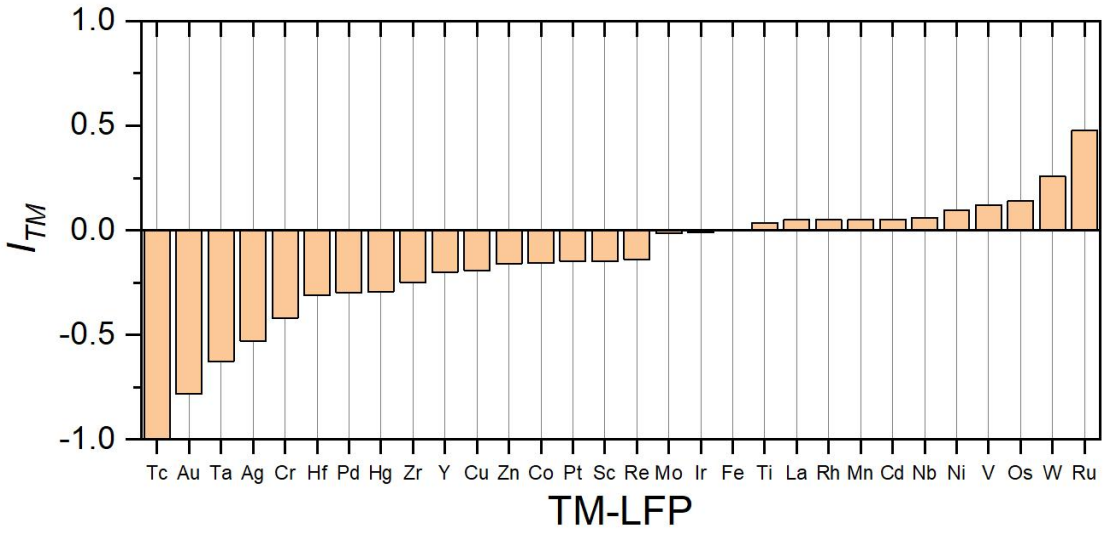
200 **Supplementary Figure 20. Anisotropy shear moduluses of the <001> and <100>**

201 **directions of {010} planes.**

202



Supplementary Figure 21. Anisotropy shear moduluses of the <110> and <010> directions of {001} planes.

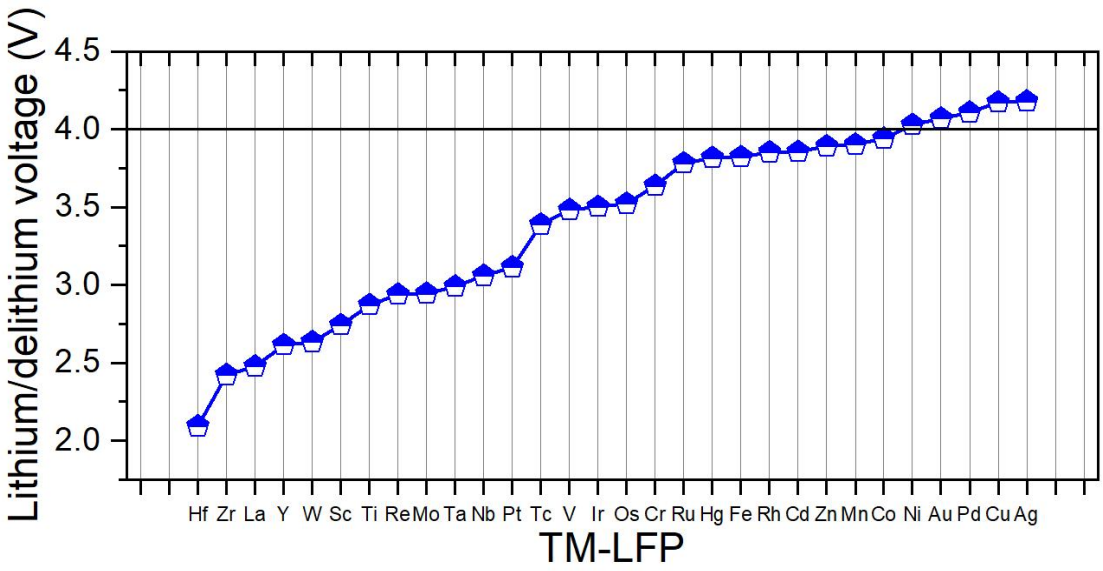


Supplementary Figure 22. Difference (I_{TM}) between TM-LFP and LFP models. $I_{TM} = A_{LFP} - A_{TM}$.

7. Screening for higher operating voltages

Supplementary Table 52. Lithium/delithium voltages of all the TM-LFP models.

Materials	Voltage (V)	Materials	Voltage (V)
Sc-$LiFePO_4$	2.7422	Ru-$LiFePO_4$	3.7809
Ti-$LiFePO_4$	2.8716	Rh-$LiFePO_4$	3.8529
V-$LiFePO_4$	3.4818	Pd-$LiFePO_4$	4.107
Cr-$LiFePO_4$	3.6367	Ag-$LiFePO_4$	4.1784
Mn-$LiFePO_4$	3.9013	Cd-$LiFePO_4$	3.8551
$LiFePO_4$	3.8212	La-$LiFePO_4$	2.4767
Co-$LiFePO_4$	3.9404	Hf-$LiFePO_4$	2.0934
Ni-$LiFePO_4$	4.0277	Ta-$LiFePO_4$	2.9902
Cu-$LiFePO_4$	4.1723	W-$LiFePO_4$	2.6338
Zn-$LiFePO_4$	3.8907	Re-$LiFePO_4$	2.9391
Y-$LiFePO_4$	2.6137	Os-$LiFePO_4$	3.5226
Zr-$LiFePO_4$	2.4222	Ir-$LiFePO_4$	3.502
Nb-$LiFePO_4$	3.0598	Pt-$LiFePO_4$	3.1141
Mo-$LiFePO_4$	2.9441	Au-$LiFePO_4$	4.0692
Tc-$LiFePO_4$	3.389	Hg-$LiFePO_4$	3.8157



Supplementary Figure 23. Lithium/delithium voltages of 30 types of TM-LFP models.

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