Supporting Information (SI)

Strain engineering of Li^+ ions migration in olivine phosphates cathode materials $LiMPO_4$ (M = Mn, Fe, Co) and $(LiFePO_4)_n(LiMnPO_4)_m$ superlattices

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Table **S1** The fitting parameters were obtained by fitting the E_b strain data of $LiMPO_4$ (M = Mn, Fe, Co) with quadratic function: $E_b = \alpha x^2 + \beta x + E_0$.

		$LiMnPO_4$			$LiFePO_4$			$LiCoPO_4$		
	strain	α	β	E_0	α	β	E_0	α	β	E_0
Path A	*ac*	0.00572	-0.11079	0.61	0.00434	-0.10015	0.54	0.00525	-0.10149	0.48
	ab	-0.00299	0.05033	0.61	-0.00283	0.04439	0.54	-0.00153	0.04739	0.48
	bc	-0.00368	0.03078	0.61	-0.00427	0.02849	0.54	-0.00363	0.0313	0.48
Path B	*ac*	-0.00483	-0.04853	2.84	-0.00823	-0.00614	2.91	-0.00983	-0.03035	3.29
	ab	-0.00486	-0.21652	2.84	-0.01004	-0.27	2.91	-0.00825	-0.2491	3.29
	bc	-0.01386	-0.07672	2.84	-0.02257	-0.11289	2.91	-0.02067	-0.1134	3.29
Path A	*a*	0	-0.03316	0.61	0	-0.03421	0.54	0	-0.03149	0.48
	b	0	0.06604	0.61	0	0.05909	0.54	0	0.06143	0.48
	c	0	-0.04168	0.61	0	-0.0381	0.54	0	-0.03599	0.48
Path B	*a*	-0.00146	-0.05139	2.84	-0.00435	-0.02535	2.91	-0.00305	-0.03669	3.29
	b	-0.00429	-0.08246	2.84	-0.00796	-0.11123	2.91	-0.00878	-0.11204	3.29
	c	-0.00346	0.02009	2.84	-0.00402	0.02518	2.91	-0.00396	0.01934	3.29

Table **S2** Comparison of the calculated superlattice volume with the ideal superlattice volume.

	Calculated volume (Å^3)	Ideal volume (Å^3)
LFP	291.4417	291.4417
SL3+1(100)	293.7849	293.7390
SL3+1(010)	293.7897	
SL3+1(001)	293.8648	
SL1+1(100)	296.0966	296.0364
SL1+1(010)	296.1290	
SL1+1(001)	296.1021	
SL1+3(100)	298.3603	298.3337
SL1+3(010)	298.3923	
SL1+3(001)	298.4556	
LMP	300.6310	300.6310

Table **S3** The fitting parameters were obtained by fitting the E_b strain data of SL3+1(100), SL3+1(010) and SL3+1(001) with quadratic function: $E_b = \alpha x^2 + \beta x + E_0$.

		SL3+1(100)			SL3+1(010)			SL3+1(001)		
	strain	α	β	E_0	α	β	E_0	α	β	E_0
Path A site 1	*ac*	0.00458	-0.10127	0.56	0.00556	-0.11179	0.62	0.00424	-0.09936	0.56
	ab	-0.00327	0.0419	0.56	-0.00316	0.04621	0.62	-0.00298	0.04658	0.56
	bc	-0.00391	0.02993	0.56	-0.00415	-0.02612	0.62	-0.00452	0.02733	0.56
	a	0	-0.03449	0.56	0	-0.03571	0.62	0	-0.03193	0.56
	b	0	0.05929	0.56	0	0.0625	0.62	0	0.05922	0.56
	c	0	-0.03719	0.56	0	-0.0429	0.62	0	-0.03886	0.56
Path A site 2	*ac*	0.00435	-0.09906	0.55	0.00405	-0.10014	0.49	0.00483	-0.10537	0.58
	ab	-0.00272	0.04435	0.55	-0.00304	0.05038	0.49	-0.00259	0.04515	0.58
	bc	-0.00413	0.02576	0.55	-0.00428	0.03279	0.49	-0.00421	0.02414	0.58
	a	0	-0.03154	0.55	0	-0.03352	0.49	0	-0.03307	0.58
	b	0	0.05786	0.55	0	0.06254	0.49	0	0.05968	0.58
	c	0	-0.03898	0.55	0	-0.03776	0.49	0	-0.04205	0.58
Path B site 1	*ac*	-0.00686	-0.01493	2.86	-0.00719	-0.01384	2.86	-0.00737	-0.02051	2.86
	ab	-0.00745	-0.25013	2.86	-0.00656	-0.25292	2.86	-0.01039	-0.267	2.86
	bc	-0.02067	-0.10541	2.86	-0.01664	-0.09411	2.86	-0.02148	-0.11862	2.86
	a	-0.00331	-0.03144	2.86	-0.0026	-0.03414	2.86	-0.00409	-0.02945	2.86
	b	-0.00696	-0.10326	2.86	-0.00493	-0.10073	2.86	-0.00746	-0.11139	2.86
	c	-0.00414	0.0243	2.86	-0.00352	0.02798	2.86	-0.00402	0.01887	2.86
Path B site 2	*ac*	-0.00747	-0.01219	2.87	-0.00865	-0.02076	2.87	-0.00838	-0.00343	2.89
	ab	-0.01055	-0.27319	2.87	-0.00919	-0.26603	2.87	-0.00901	-0.27697	2.89
	bc	-0.02269	-0.12422	2.87	-0.02141	-0.10745	2.87	-0.02123	-0.11605	2.89
	a	-0.00438	-0.02743	2.87	-0.00364	-0.03414	2.87	-0.00346	-0.02758	2.89
	b	-0.00771	-0.11755	2.87	-0.00763	-0.10664	2.87	-0.00701	-0.11878	2.89
	c	-0.00394	0.02216	2.87	-0.00315	0.02471	2.87	-0.00402	0.02916	2.89

Table **S4** The fitting parameters were obtained by fitting the E_b strain data of SL1+1(100), SL1+1(010) and SL1+1(001) with quadratic function: $E_b = \alpha x^2 + \beta x + E_0$.

		SL1+1(100)			SL1+1(010)			SL1+1(001)		
	strain	α	β	E_0	α	*B*	E_0	α	β	E_0
Path A	*ac*	0.00415	-0.09938	0.57	0.00548	-0.10997	0.56	0.00442	-0.10683	0.60
	ab	-0.0034	0.04183	0.57	-0.00257	0.05332	0.56	-0.00361	0.04906	0.60
	bc	-0.00395	0.02736	0.57	-0.00346	0.03047	0.56	-0.00487	0.02374	0.60
	a	0	-0.03245	0.57	0	-0.034	0.56	0	-0.03129	0.60
	b	0	0.05824	0.57	0	0.06608	0.56	0	0.0609	0.60
	c	0	-0.03771	0.57	0	-0.04272	0.56	0	-0.04359	0.60
Path B	*ac*	-0.00687	-0.0217	2.83	-0.00824	-0.02413	2.83	-0.00864	-0.01996	2.86
	ab	-0.00768	-0.25174	2.83	-0.00745	-0.25129	2.83	-0.00989	-0.27287	2.86
	bc	-0.02133	-0.11576	2.83	-0.01769	-0.09426	2.83	-0.02034	-0.11764	2.86
	a	-0.00357	-0.03281	2.83	-0.00332	-0.04093	2.83	-0.00409	-0.03358	2.86
	b	-0.00693	-0.10841	2.83	-0.00624	-0.10079	2.83	-0.00716	-0.11791	2.86

	c	-0.00447	0.02042	2.83	-0.0044	0.02635	2.83	-0.00461	0.02213	2.86

Table **S5** The fitting parameters were obtained by fitting the E_b strain data of SL1+3(100), SL1+3(010) and SL1+3(001) with quadratic function: $E_b = \alpha x^2 + \beta x + E_0$.

		SL3+1(100)			SL3+1(010)			SL3+1(001)		
	strain	α	β	E_0	α	β	E_0	α	β	E_0
Path A site 1	*ac*	0.00553	-0.11076	0.60	0.00483	-0.10115	0.54	0.00566	-0.11057	0.60
	ab	-0.00249	0.05437	0.60	-0.00267	0.05045	0.54	-0.00254	0.04921	0.60
	bc	-0.00394	0.02938	0.60	-0.00401	0.03556	0.54	-0.00385	0.03079	0.60
	a	0	-0.03243	0.60	0	-0.03267	0.54	0	-0.03445	0.60
	b	0	0.06611	0.60	0	0.0644	0.54	0	0.06532	0.60
	c	0	-0.04327	0.60	0	-0.03661	0.54	0	-0.04058	0.60
Path A site 2	*ac*	0.00618	-0.11238	0.60	0.00569	-0.11323	0.66	0.00559	-0.10345	0.57
	ab	-0.00294	0.0507	0.60	-0.00348	0.04343	0.66	-0.00207	0.04966	0.57
	bc	-0.0037	0.03248	0.60	-0.00435	0.02613	0.66	-0.00338	0.03332	0.57
	a	0	-0.03484	0.60	0	-0.03474	0.66	0	-0.03265	0.57
	b	0	0.06636	0.60	0	0.06232	0.66	0	-0.06375	0.57
	c	0	-0.04149	0.60	0	-0.04217	0.66	0	-0.03679	0.57
Path B site 1	*ac*	-0.00624	-0.02807	2.80	-0.00807	-0.03479	2.81	-0.00509	-0.03541	2.85
	ab	-0.00774	-0.25305	2.80	-0.00709	-0.24803	2.81	-0.00444	-0.22148	2.85
	bc	-0.02132	-0.12435	2.80	-0.01721	-0.09035	2.81	-0.01427	-0.07361	2.85
	a	-0.00378	-0.03466	2.80	-0.00286	-0.04819	2.81	-0.00096	-0.04749	2.85
	b	-0.00652	-0.11276	2.80	-0.00612	-0.09759	2.81	-0.00416	-0.08305	2.85
	c	-0.00412	0.01744	2.80	-0.00366	0.02615	2.81	-0.00339	0.02521	2.85
Path B site 2	*ac*	-0.00537	-0.04209	2.86	-0.00481	-0.0433	2.86	-0.00438	-0.05204	2.83
	ab	-0.00504	-0.21508	2.86	-0.00523	-0.21811	2.86	-0.00587	-0.21311	2.83
	bc	-0.0144	-0.07145	2.86	-0.01416	-0.07656	2.86	-0.01459	-0.07581	2.83
	a	-0.00184	-0.04922	2.86	-0.00136	-0.04778	2.86	-0.00164	-0.04932	2.83
	b	-0.00492	-0.08015	2.86	-0.00427	-0.08206	2.86	-0.00474	-0.07608	2.83
	c	-0.00416	0.02213	2.86	-0.00367	0.01938	2.86	-0.00331	0.01617	2.83