Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

High Throughput Finding Li Ion Diffusion Pathway in Typical Solid State Electrolytes and Electrode Materials by BV-Ewald Method

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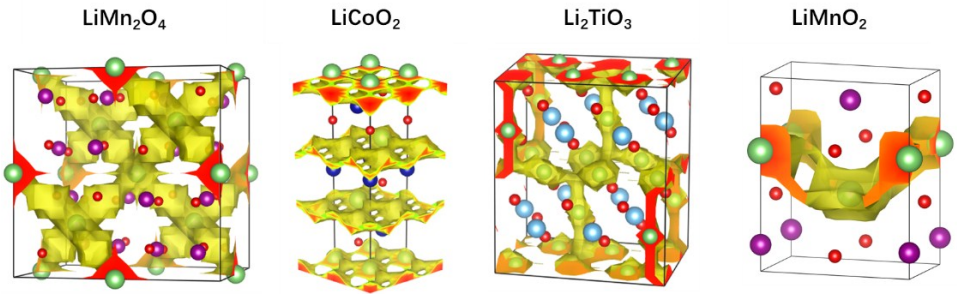
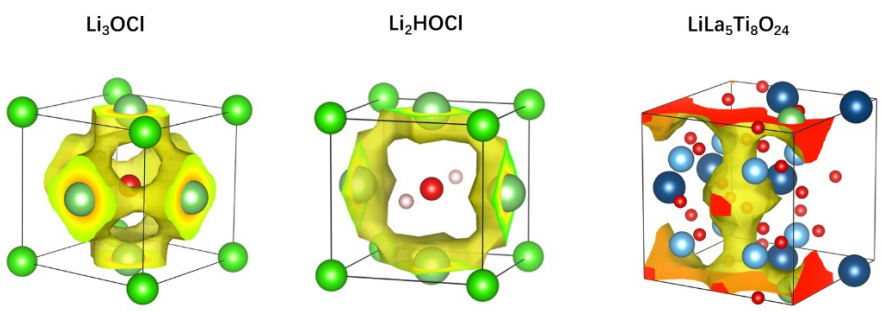
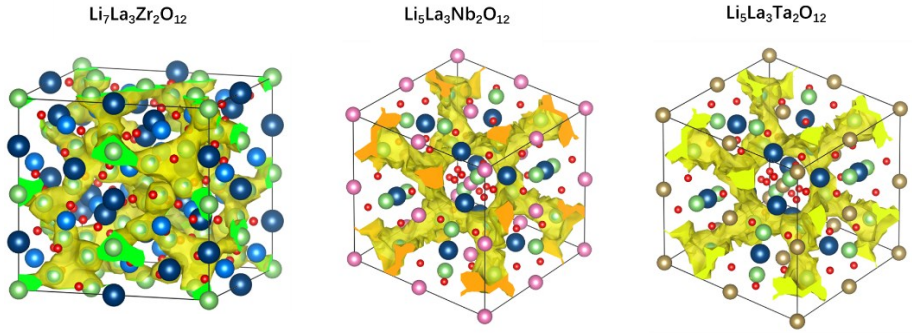
(a)Electrode Materials



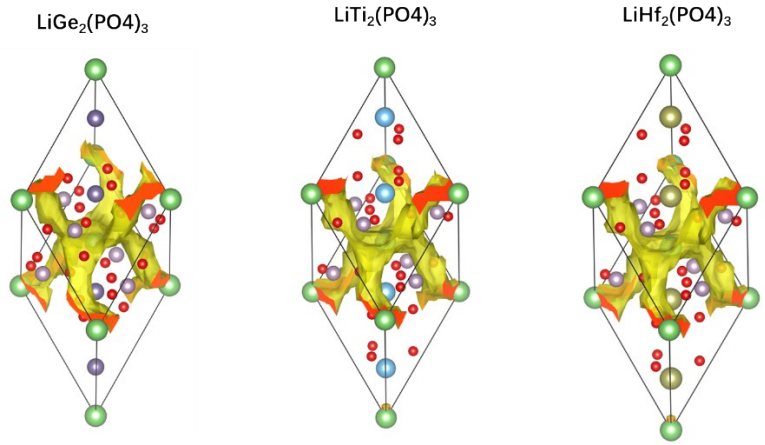
(b) (anti)perovskite



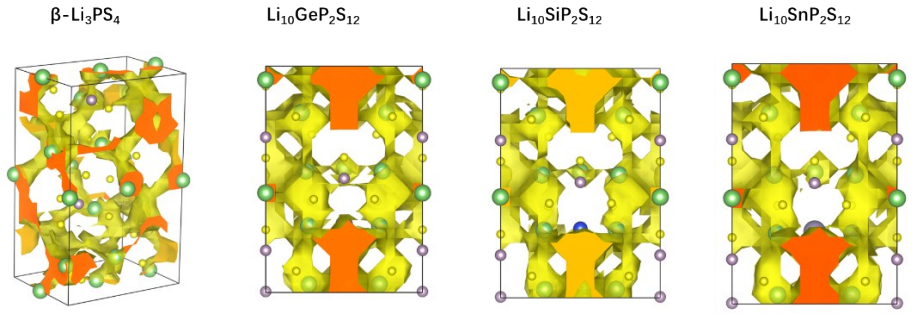
(c) Garnet



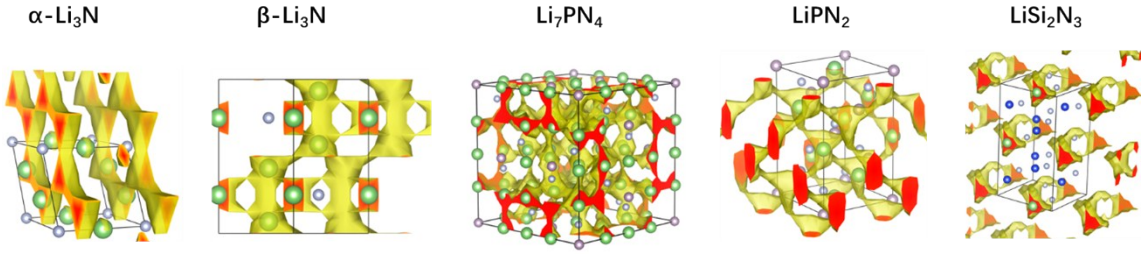
(d) NASICON



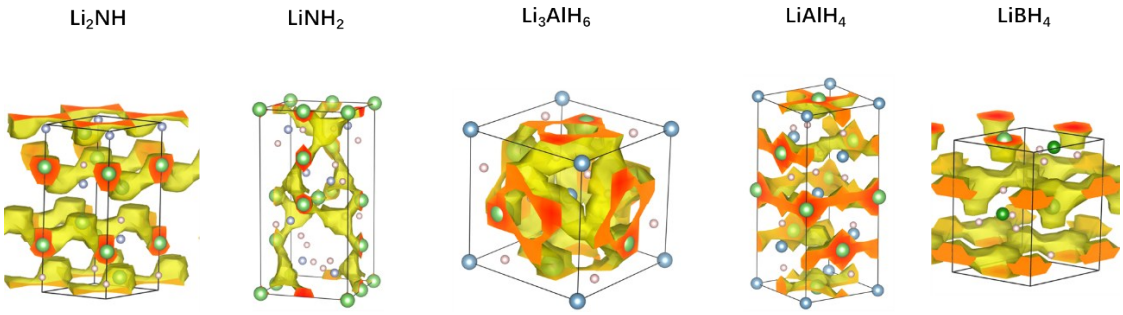
(e) LISICON



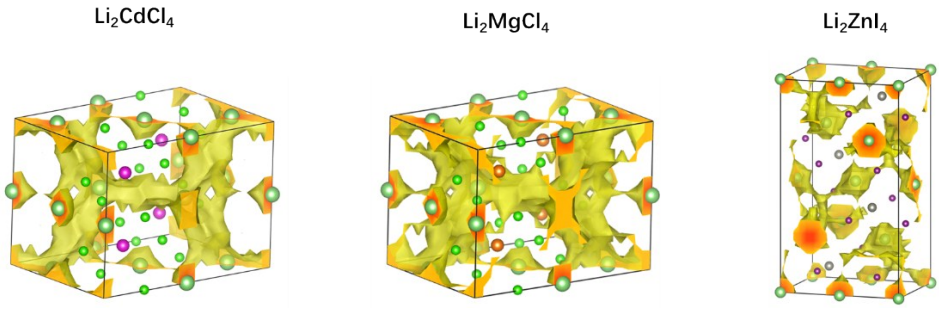
(f) Li-nitride



(g) Li-hydride



(h) Li-Halide



(i) Argyrodite

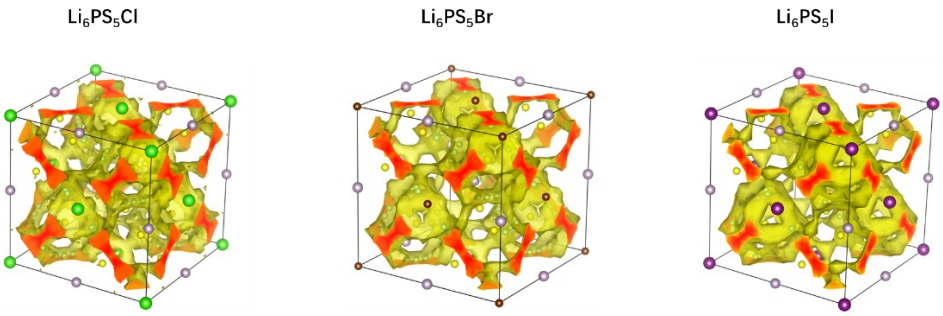


Figure S1. The Li ion diffusion map of typical electrode materials and solid state electrolytes. (a) $LiMn_2O_4$, $LiCo_2O_2$, Li_2TiO_3, $LiMnO_2$; (b) Li_3OCl, Li_2OHCl, $LiLa_5Ti8O_{24}$; (c) $Li_7La_3Zr_2O_{12}$, $Li_5La_3Nb_2O_{12}$, $Li_5La_3Ta_2O_{12}$; (d) $LiTi_2(PO_4)_3$, $LiGe_2(PO_4)_3$, $LiHf_2(PO_4)_3$; (e) β-Li_3PS_4, $Li_{10}GeP_2S_{12}$, $Li_{10}SiP_2S_{12}$,$Li_{10}SnP_2S_{12}$; (f) α-Li_3N, β-Li_3N, Li_7PN_4, $LiPN_2$, $LISi_2N_3$; (g) Li_2HN, LiH_2N, $LiBH_4$, Li_3AlH_6, $LIAlH_4$; (i) Li_2CdCl_4, Li_2MgCl_4, Li_2ZnI_4; (i) Li_6PS_5Br, Li_6PS_5Cl, Li_6PS_5I.

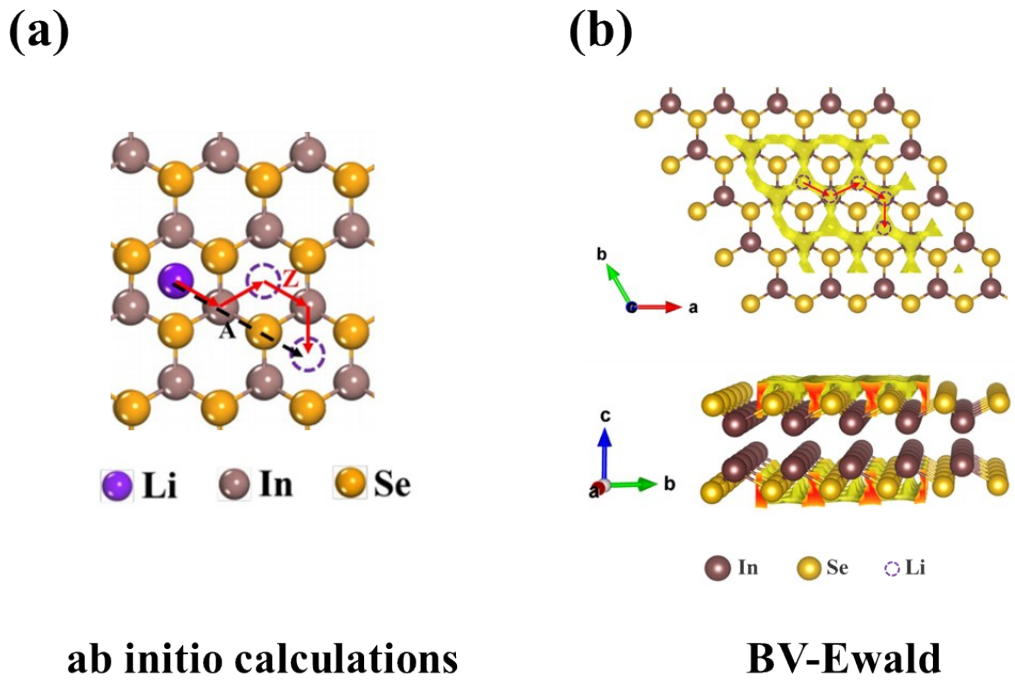


Figure S2 (a) The Li ion diffusion pathway of 2D InSe calculated by ab initio calculation. (reproduced from *Adsorption and Diffusion of Lithium on Layered InSe, ACS Omega, peer-review, Manuscript ID: ao-2018-031976*) (b) The Li ion diffusion pathway of 2D InSe calculated by BV-Ewald method.