

Supplementary information[†]

Novel fast Li-ion conductors for solid-state electrolytes from first-principles

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The following sections exhaustively illustrate the MSD plots derived from FPMD simulations of all the structures discussed in the main text.

S1 Fast Li-ion conductors

We discover 9 novel fast Li-ion conductors that exhibit significant diffusion at low temperatures along with desirable activation energy. We show the MSD plots at 1000 K, 750 K, 600 K and 500 K.

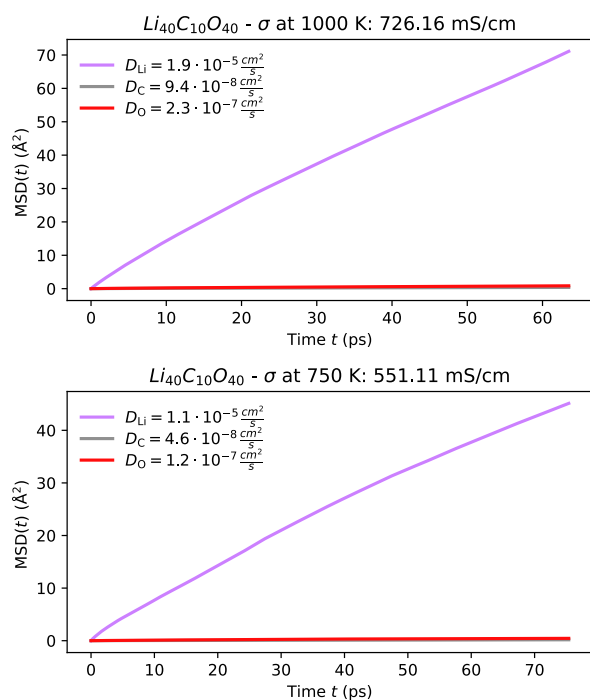


Fig. S1 MSD(t) plot of Li along with host-lattice species of Li_4CO_4 at all temperatures studied with FPMD.

We show the iso-surface plots at 600 K for the oxides and nitride.

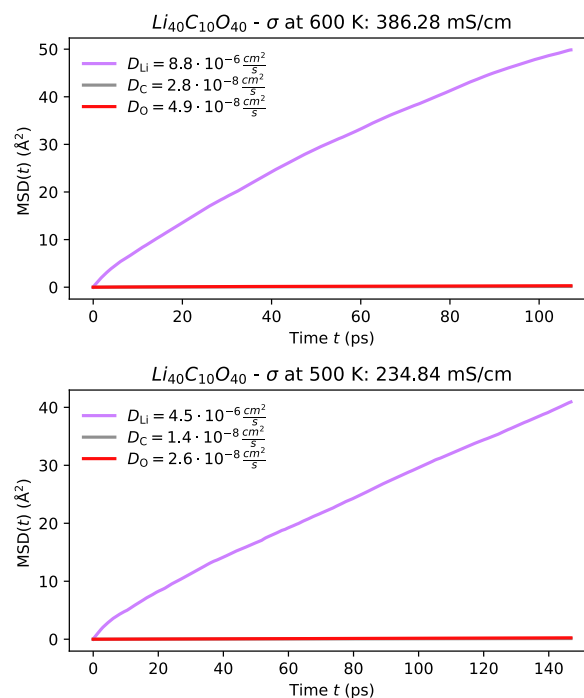


Fig. S2 MSD(t) plot of Li along with host-lattice species of Li_4CO_4 at all temperatures studied with FPMD.

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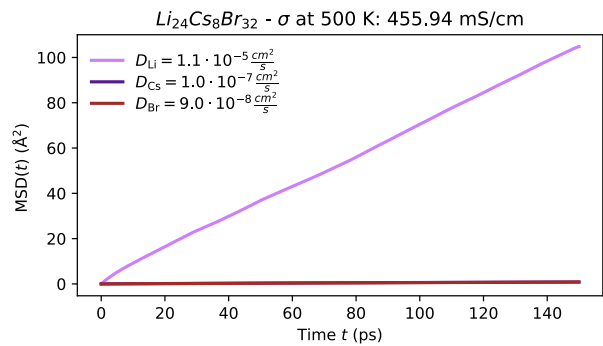
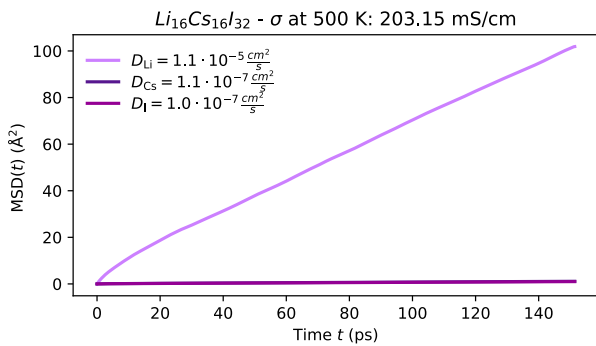
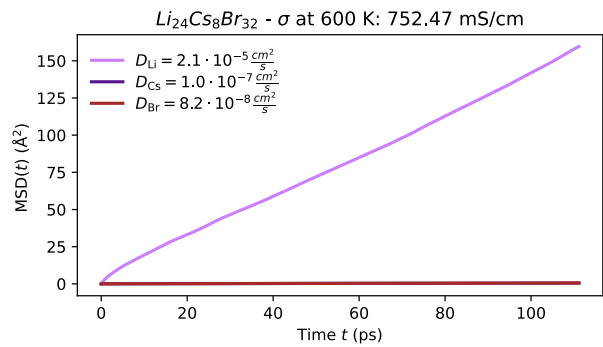
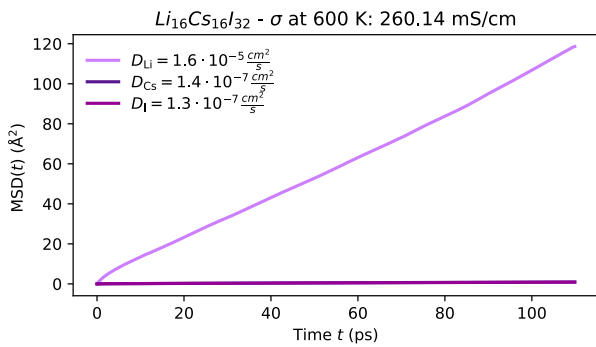
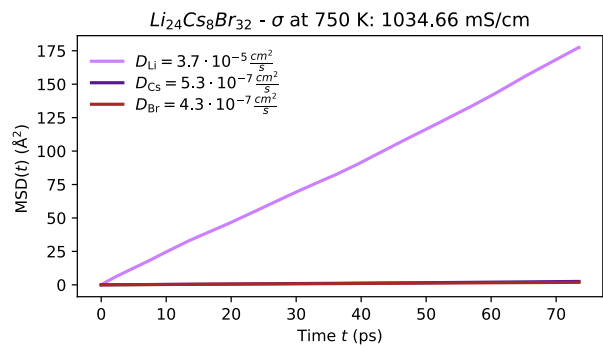
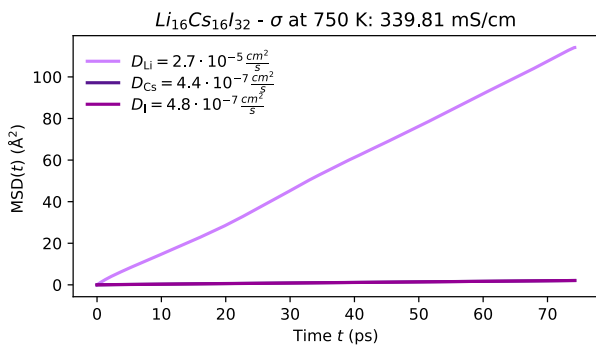
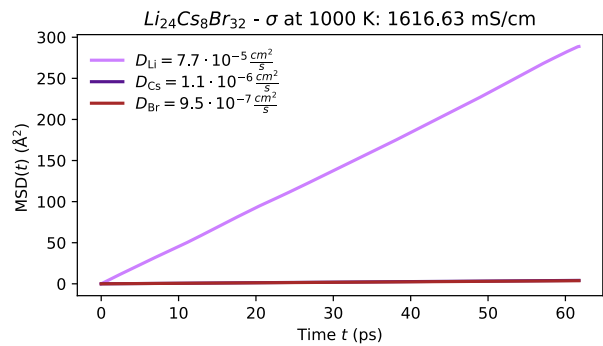
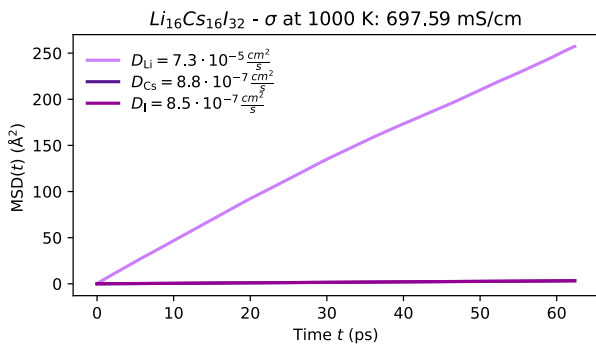


Fig. S3 MSD(t) plot of Li along with host-lattice species of *LiCsI₂* at all temperatures studied with FPMD.

Fig. S4 MSD(t) plot of Li along with host-lattice species of *Li₃CsBr₄* at all temperatures studied with FPMD.

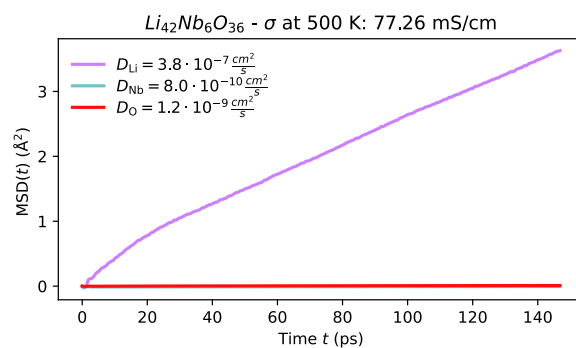
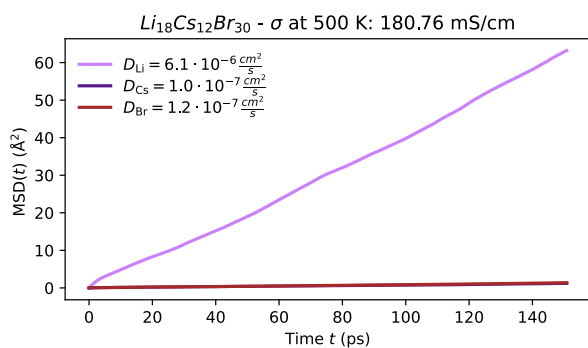
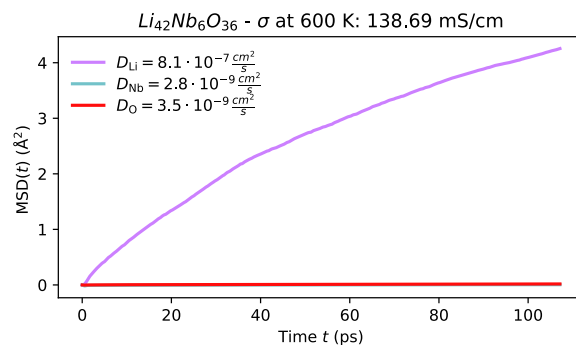
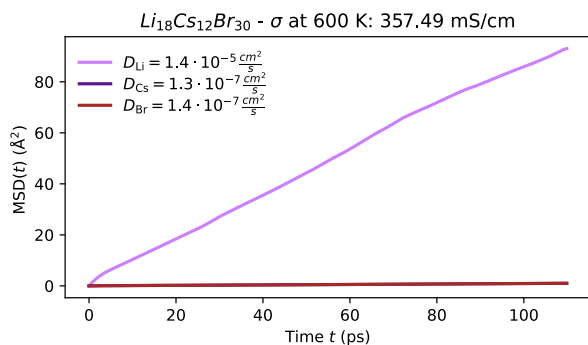
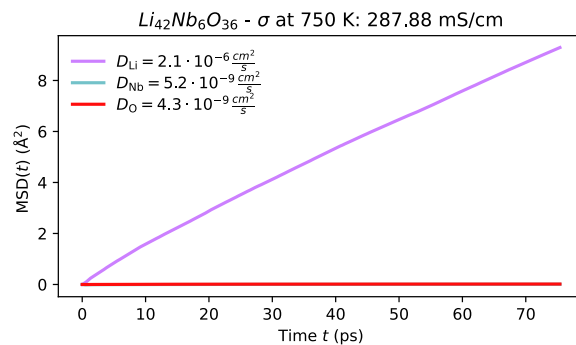
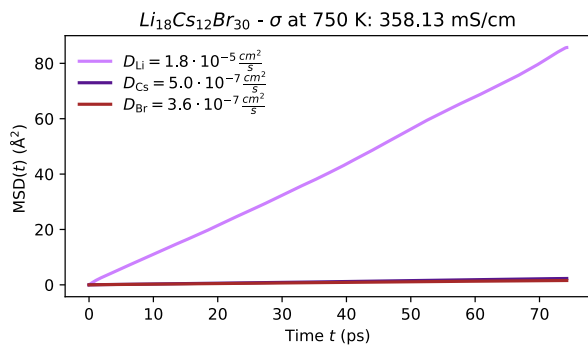
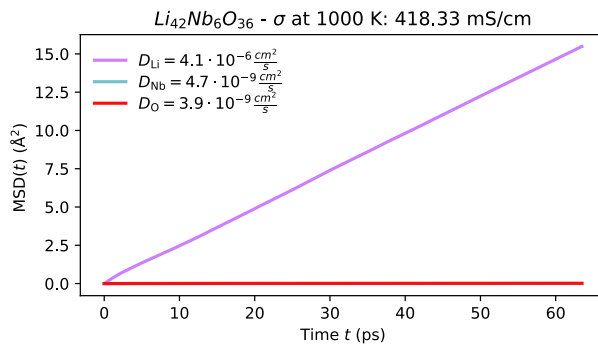
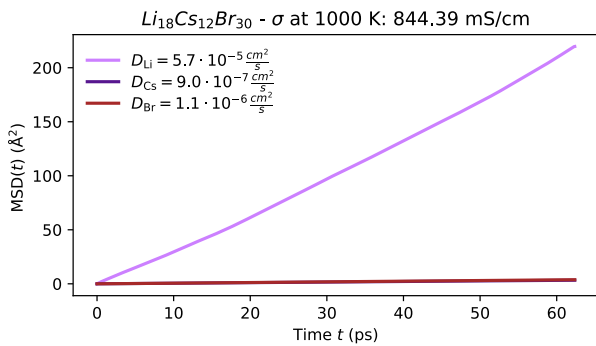


Fig. S5 MSD(t) plot of Li along with host-lattice species of *Li₁₈Cs₁₂Br₃₀* at all temperatures studied with FPMD.

Fig. S6 MSD plot of Li along with host-lattice species of *Li₄₂Nb₆O₃₆* at all temperatures studied with FPMD

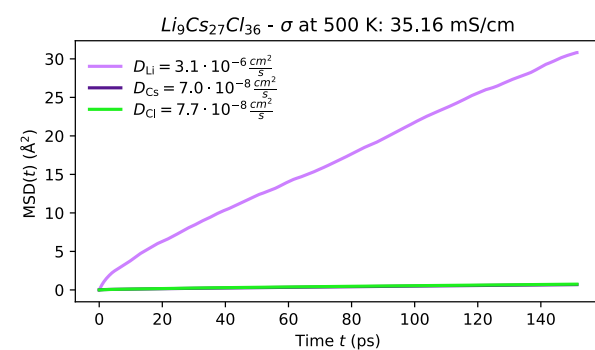
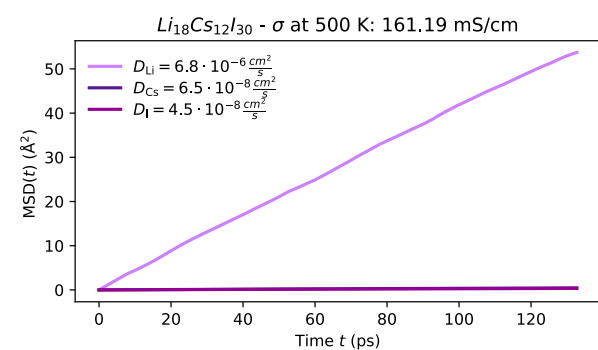
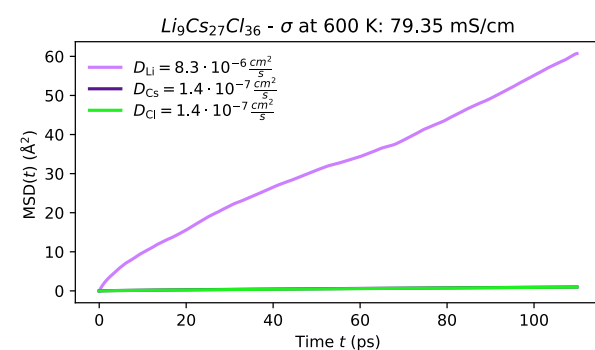
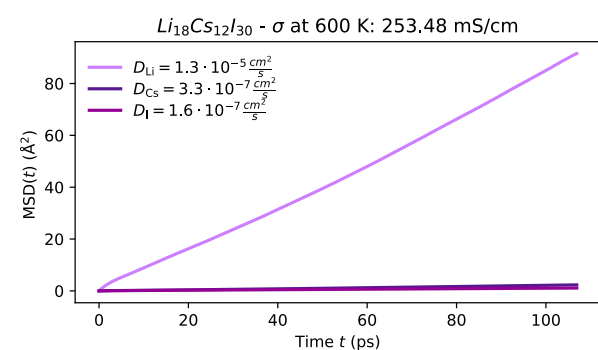
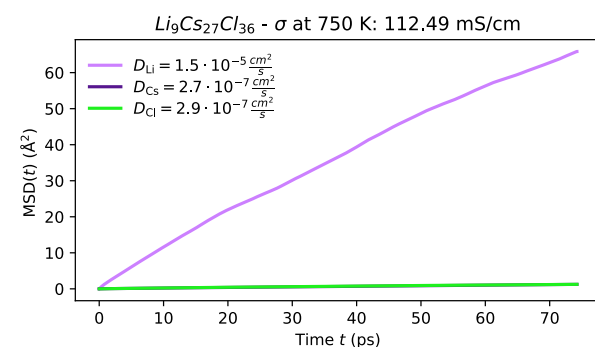
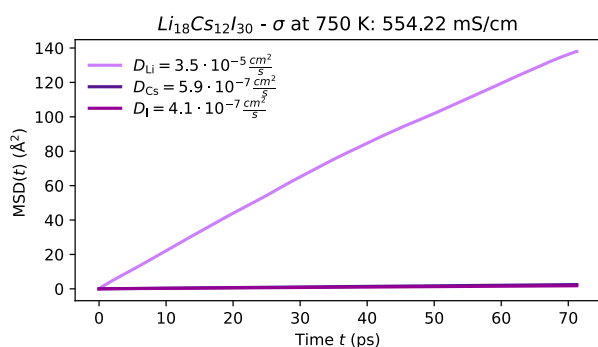
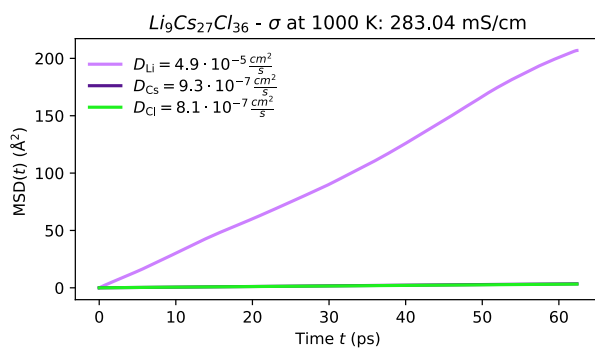
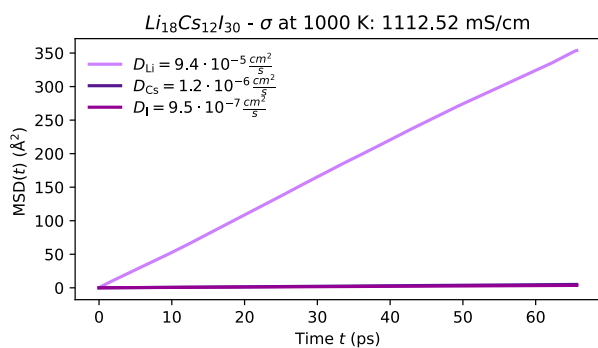


Fig. S7 MSD plot of Li along with host-lattice species of *Li₃CS₂I₅* at all temperatures studied with FPMD

Fig. S8 MSD plot of Li along with host-lattice species of *LiCS₃Cl₄* at all temperatures studied with FPMD

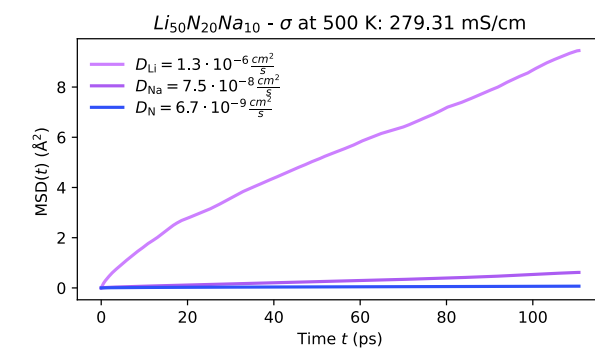
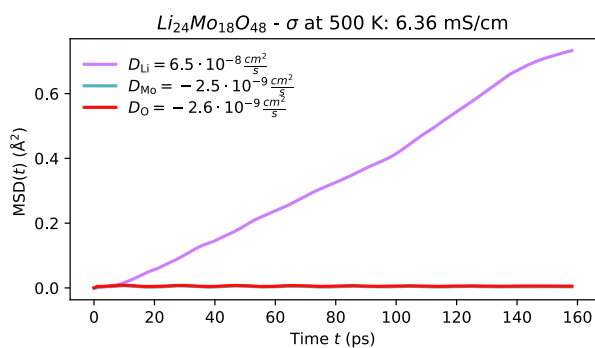
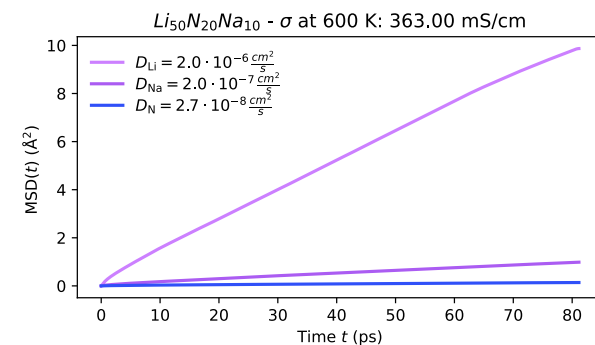
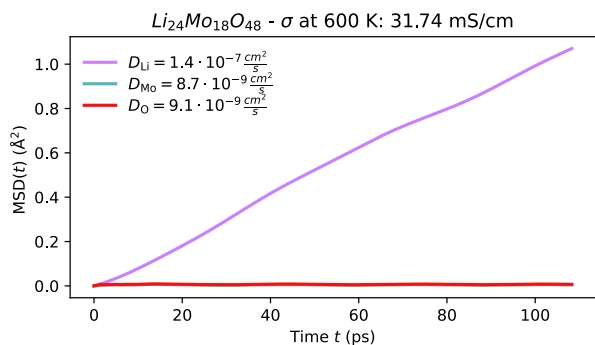
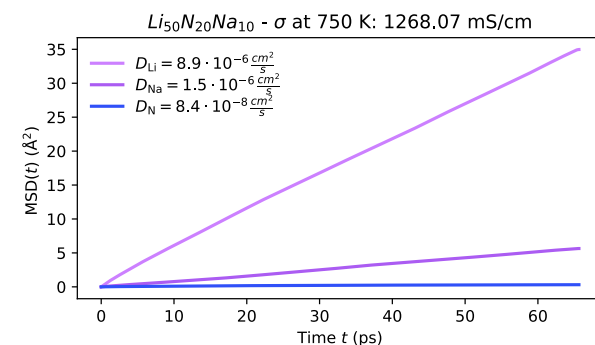
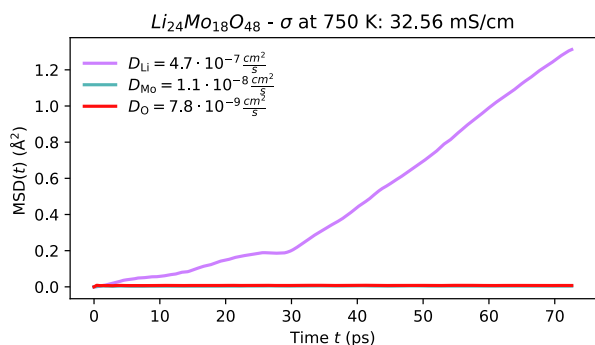
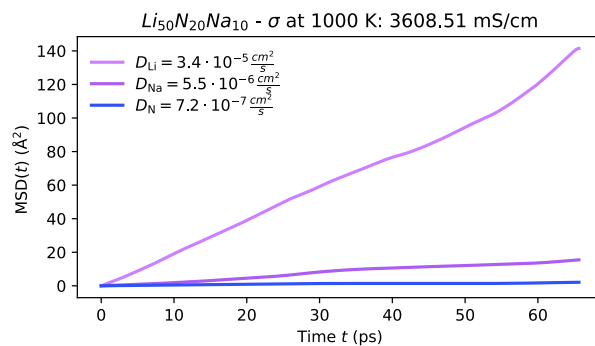
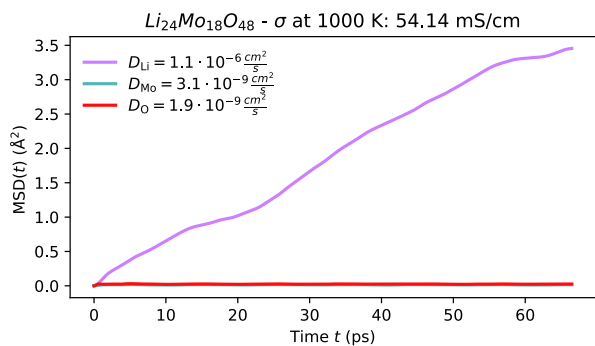


Fig. S9 MSD plot of Li along with host-lattice species of *Li₄Mo₃O₈* at all temperatures studied with FPMD

Fig. S10 MSD plot of Li along with host-lattice species of *Li₅NaN₂* at all temperatures studied with FPMD

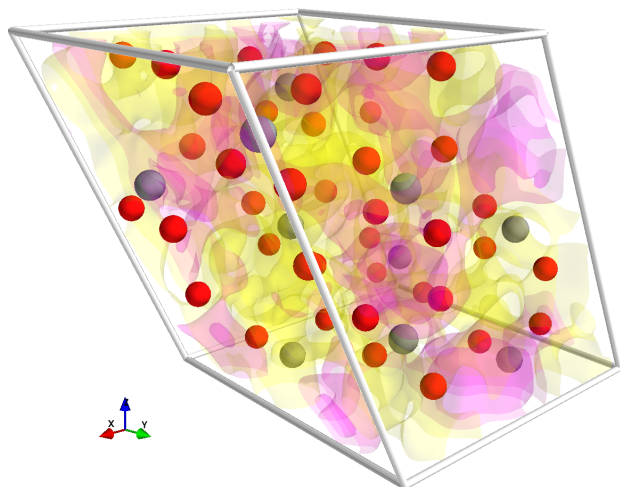


Fig. S11 Li-ion density of Li_4CO_4 at 600 K from FPMD. The pink and yellow channels clearly illustrate Li-ion diffusion in this material, establishing this materials as a 3-dimensional Li-ion conductor even at lower temperatures.

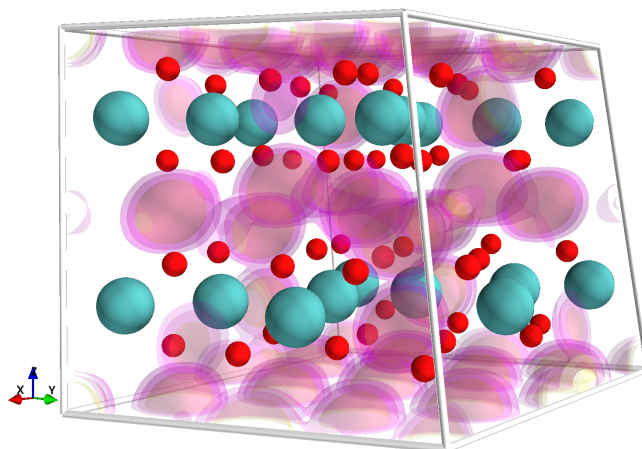


Fig. S13 Li-ion density of $Li_4M_{03}O_8$ at 600 K from FPMD. The pink clouds illustrate Li-ion diffusion in this material in a layered fashion, establishing this materials as a 3-dimensional Li-ion conductor even at lower temperatures.

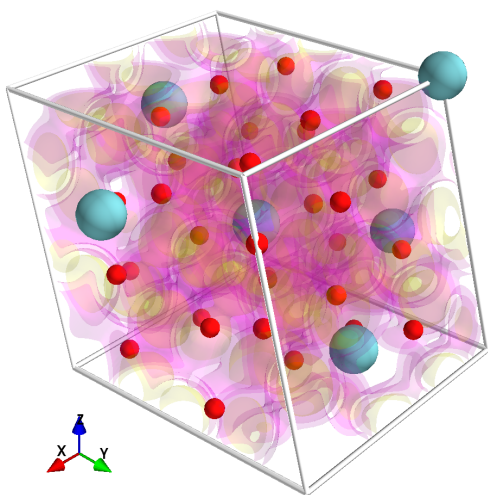


Fig. S12 Li-ion density of Li_7NbO_6 at 600 K from FPMD. The pink and yellow clouds depict Li-ion diffusion in a dispersed manner, establishing this materials as a robust 3-dimensional ionic conductor at lower temperatures.

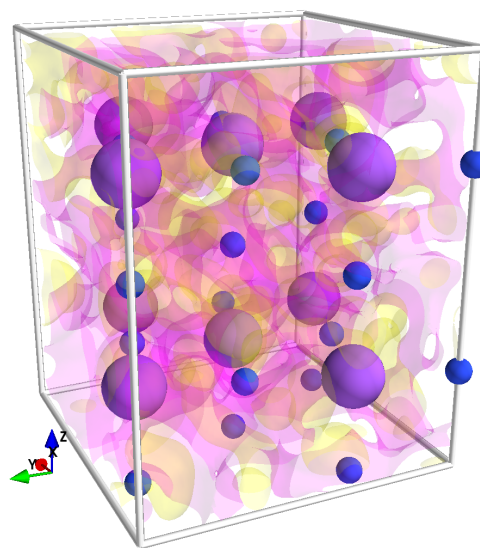


Fig. S14 Li-ion density of Li_5NaN_2 at 600 K from FPMD. The pink and yellow clouds illustrate Li-ion diffusion in a dispersed fashion, establishing this materials as a promising 3-dimensional ionic conductor at lower temperatures.

S2 Potential fast Li-ion conductors

We identify 25 structures that exhibit significant diffusion at 1000 K in our FPMD simulations, but do not display the same behaviour at lower temperatures. We show the MSD plots at 1000 K, 750 K, 600 K and 500 K.

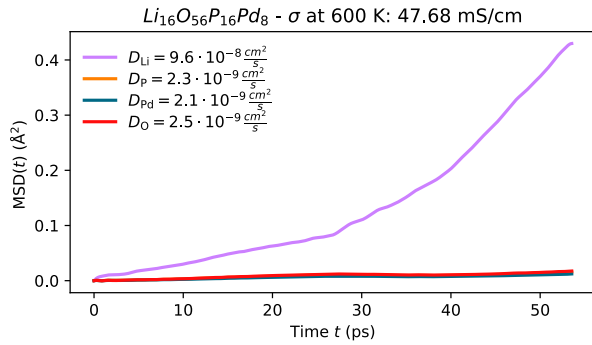


Fig. S15 MSD plot of Li along with host-lattice species of *Li₂P₂PdO₇* at 600 K. This structure was too expensive to simulate with full-first principles so we studied it at only 600 K with FPMD.

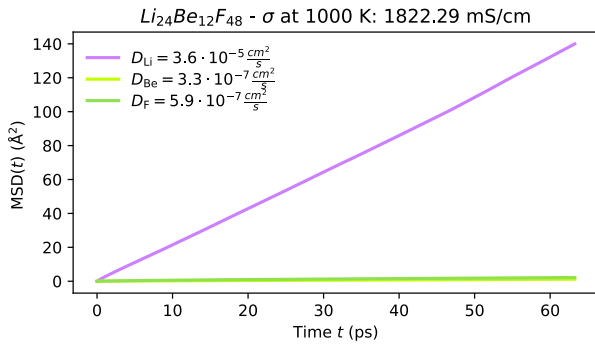


Fig. S16 MSD(t) plot of Li along with host-lattice species of *Li₂BeF₄* at 1000 K, studied with FPMD.

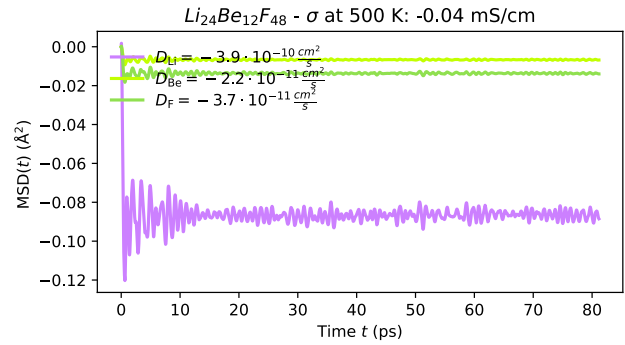
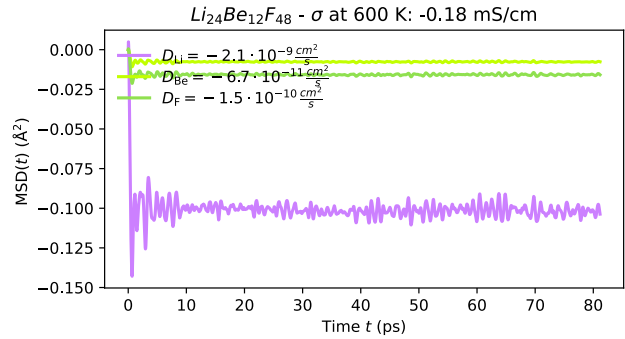
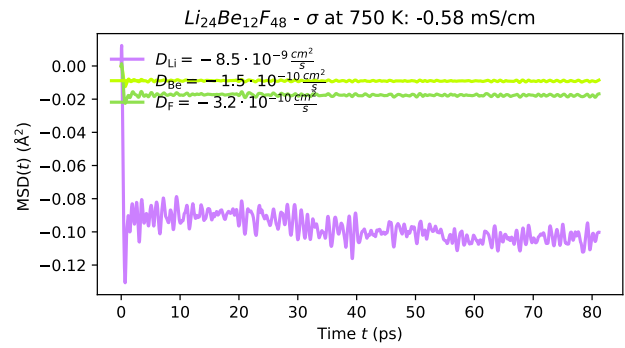


Fig. S17 MSD plot of Li along with host-lattice species of *Li₂BeF₄* at 750 K, 600 K, and 500 K, studied with FPMD

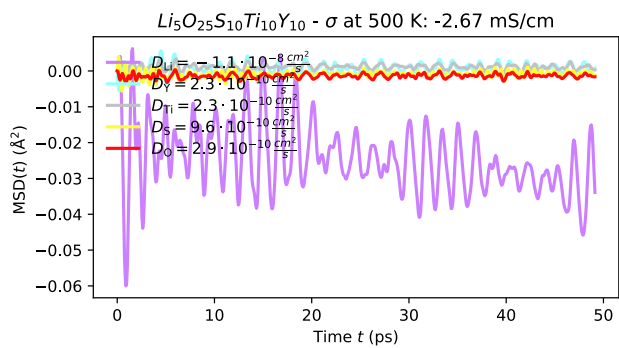
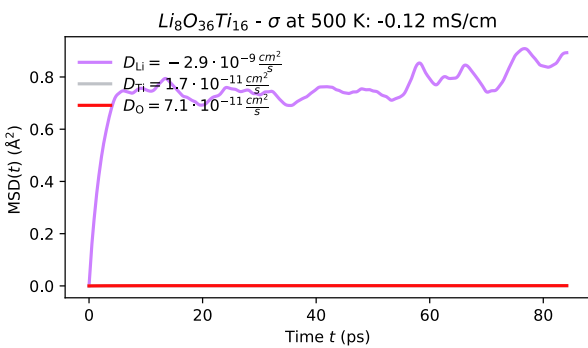
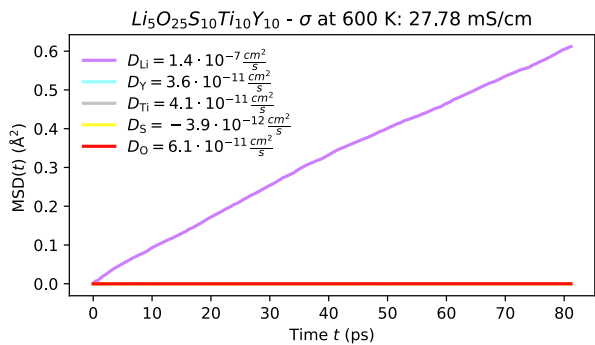
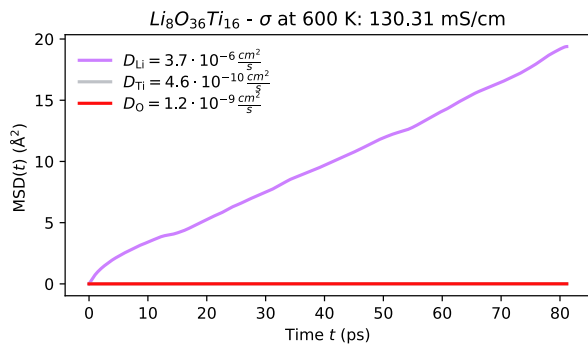
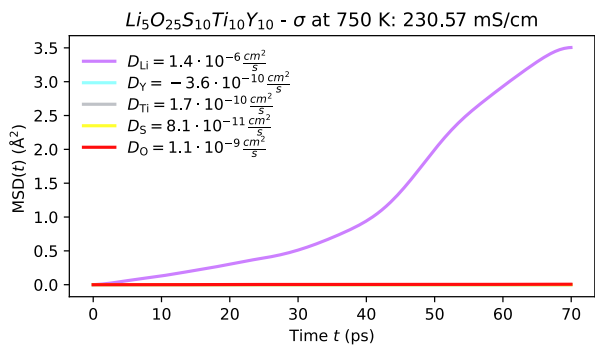
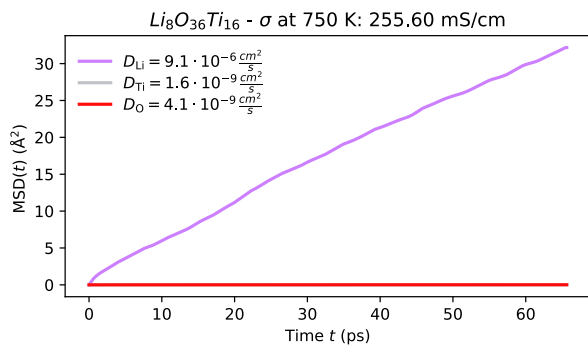
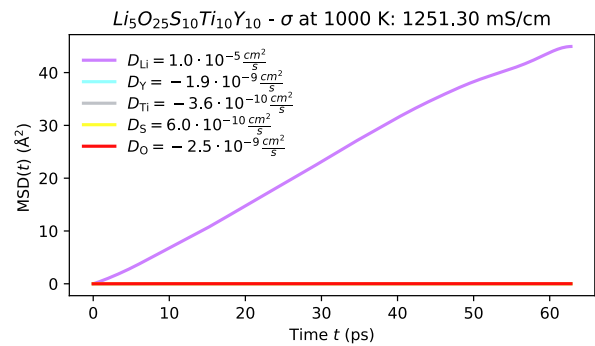
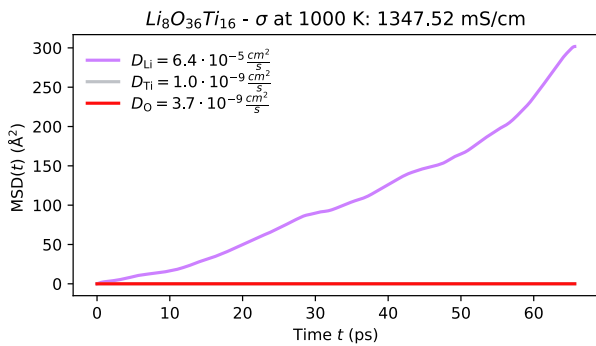


Fig. S18 MSD plot of Li along with host-lattice species of $\text{Li}_2\text{Ti}_4\text{O}_9$ at all temperatures studied with FPMD

Fig. S19 MSD plot of Li along with host-lattice species of $\text{LiY}_2\text{Ti}_2\text{S}_2\text{O}_5$ at all temperatures studied with FPMD

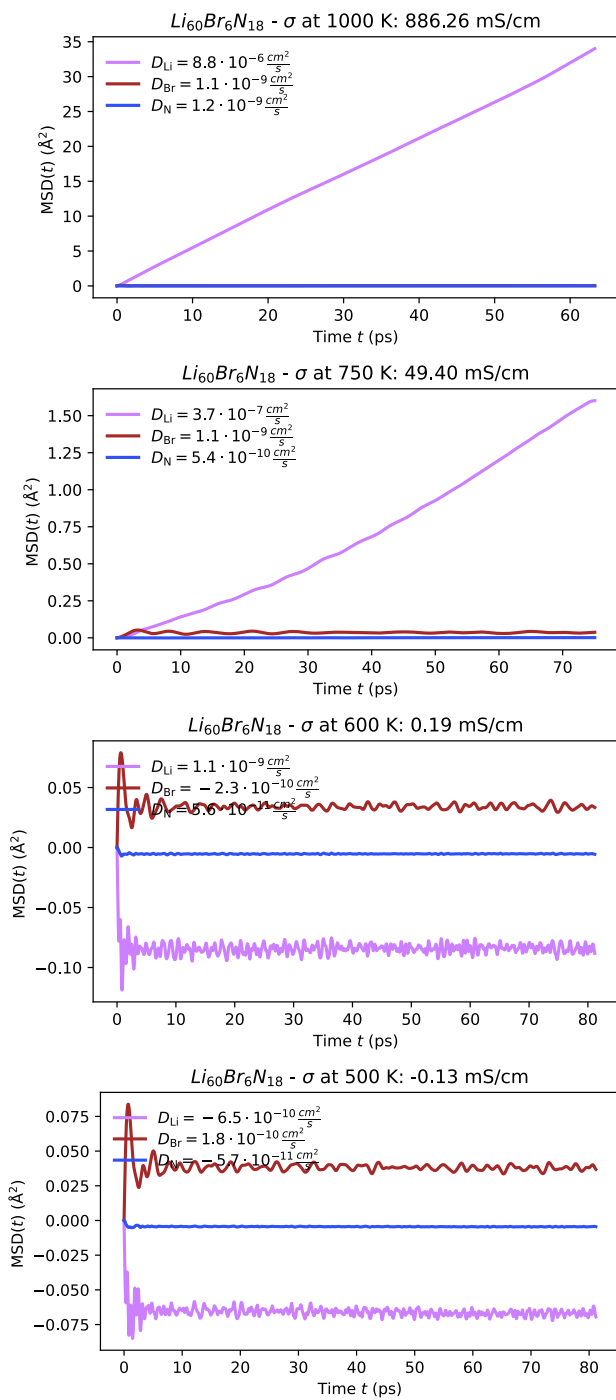


Fig. S20 MSD plot of Li along with host-lattice species of Li_1OBrN_3 at all temperatures studied with FPMD

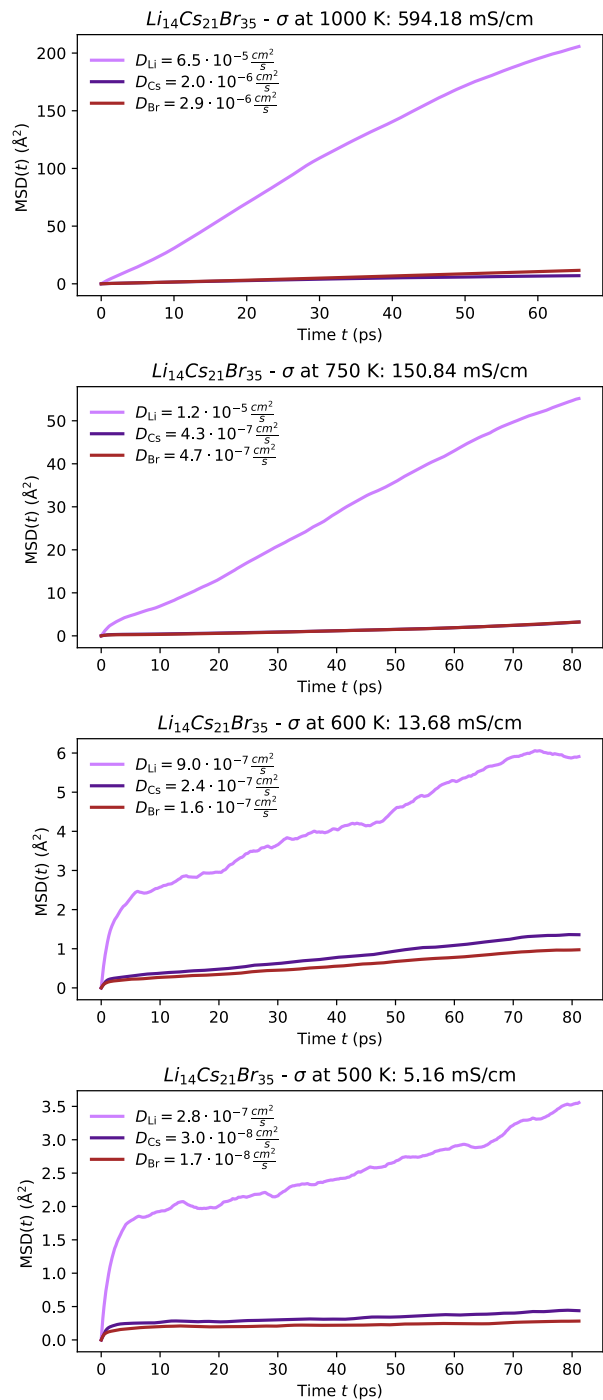


Fig. S21 MSD plot of Li along with host-lattice species of $\text{Li}_2\text{Cs}_3\text{Br}_5$ at all temperatures studied with FPMD

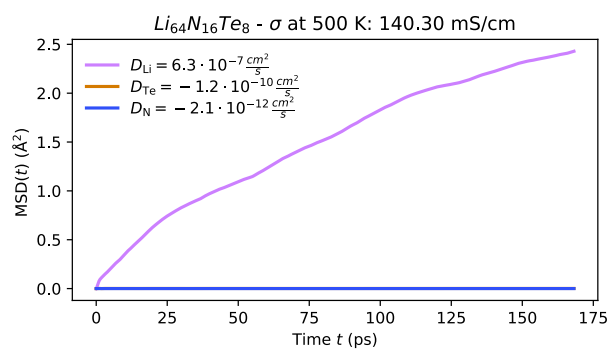
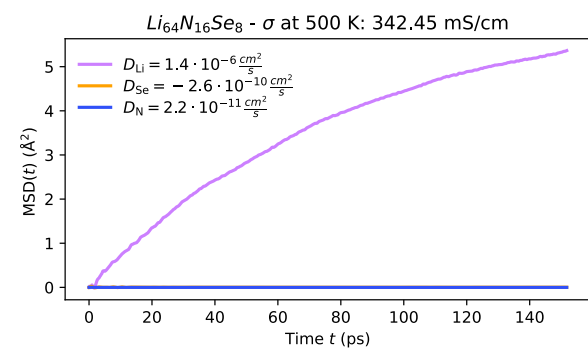
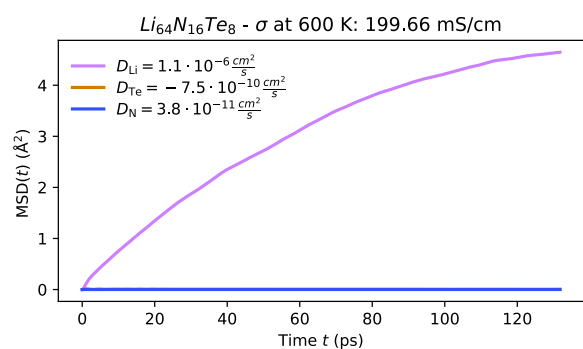
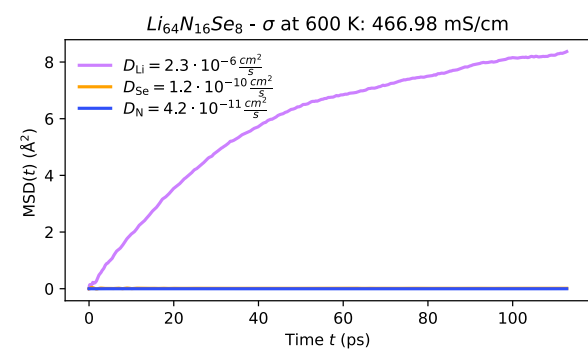
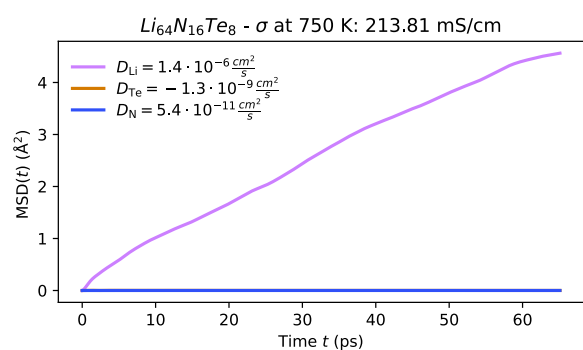
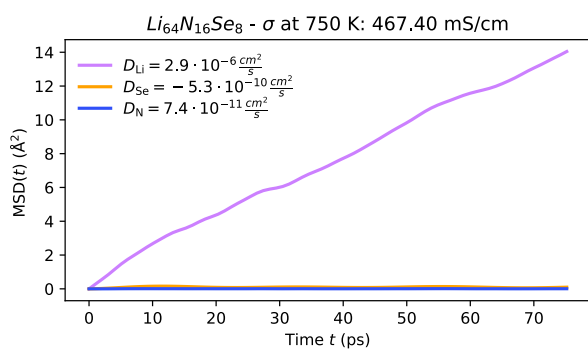
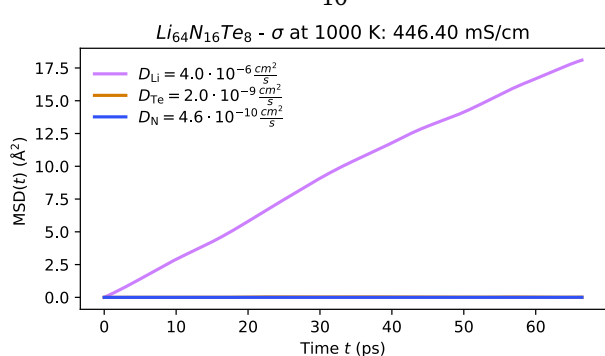
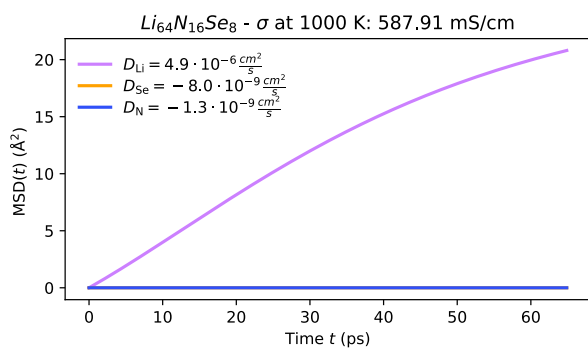


Fig. S22 MSD(t) plot of Li along with host-lattice species of *Li₈SeN₂* at all temperatures studied with FPMD.

Fig. S23 MSD(t) plot of Li along with host-lattice species of *Li₈TeN₂* at all temperatures studied with FPMD.

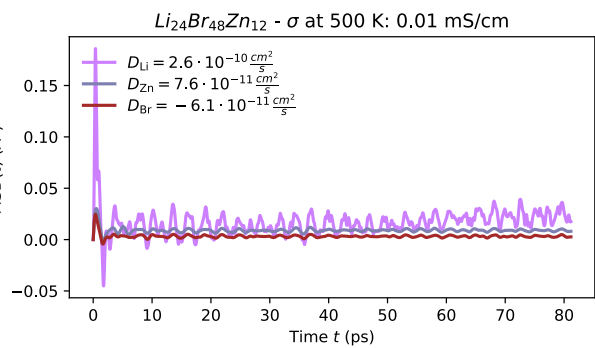
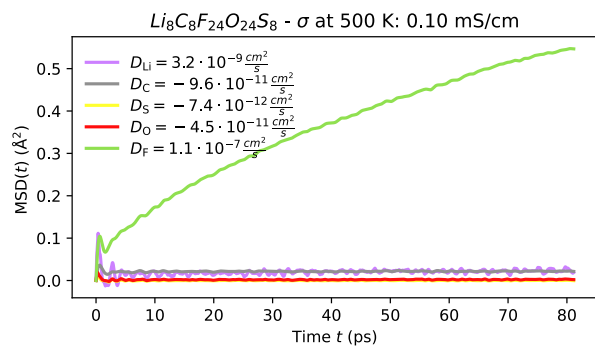
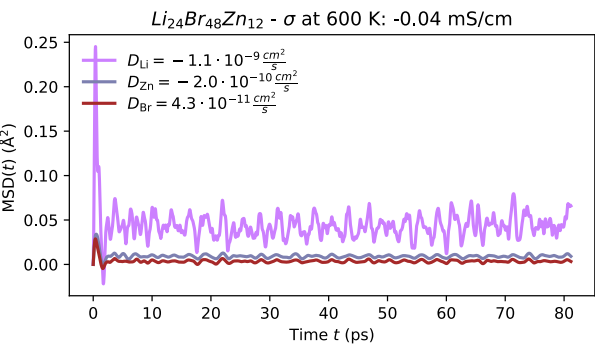
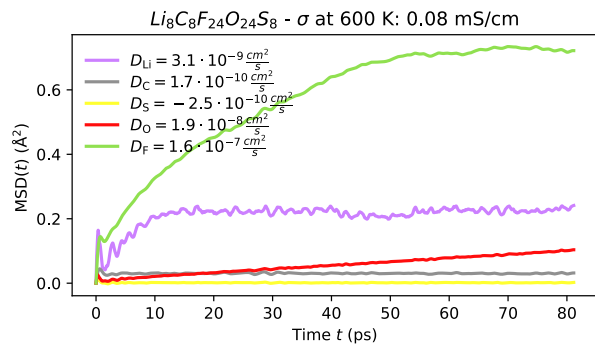
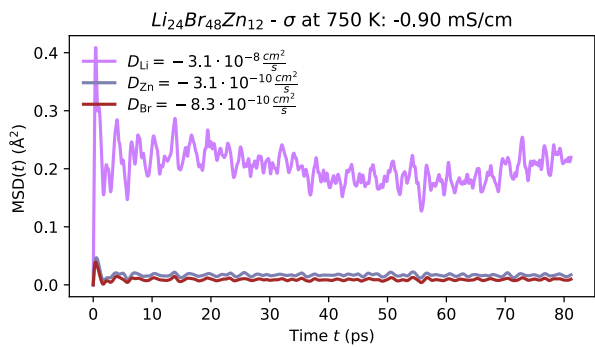
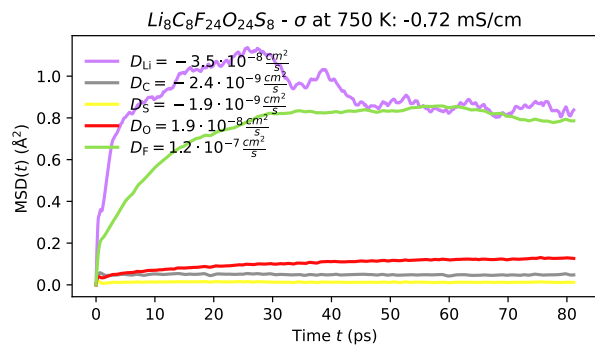
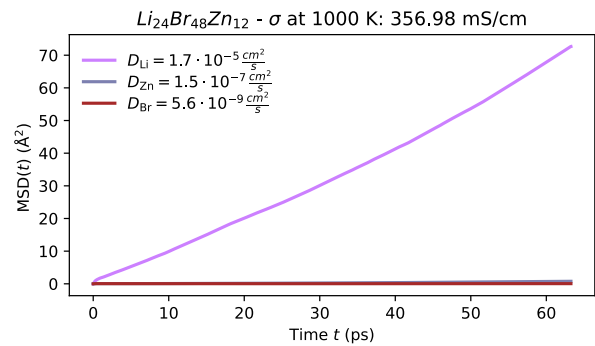
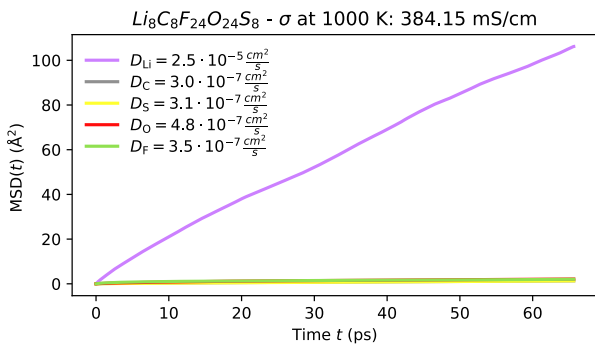


Fig. S24 MSD plot of Li along with host-lattice species of *LiCS(OF)₃* at all temperatures studied with FPMD

Fig. S25 MSD plot of Li along with host-lattice species of *Li₂ZnBr₄* at all temperatures studied with FPMD

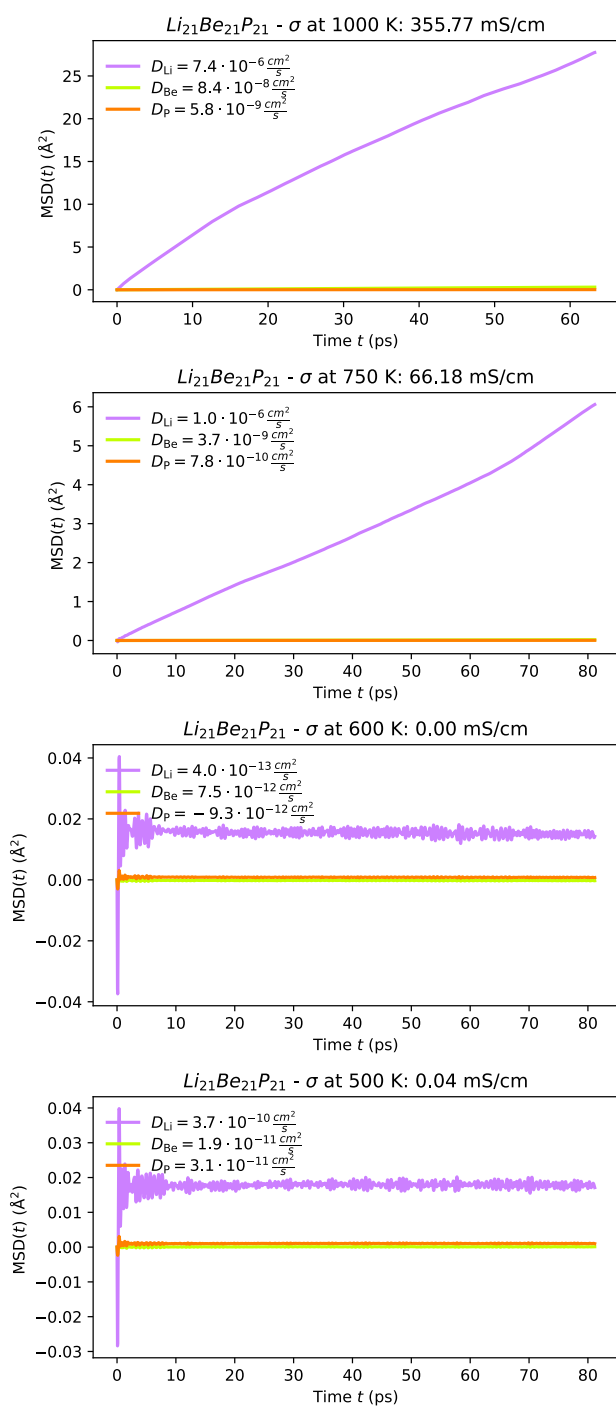


Fig. S26 MSD plot of Li along with host-lattice species of *LiBeP* at all temperatures studied with FPMD

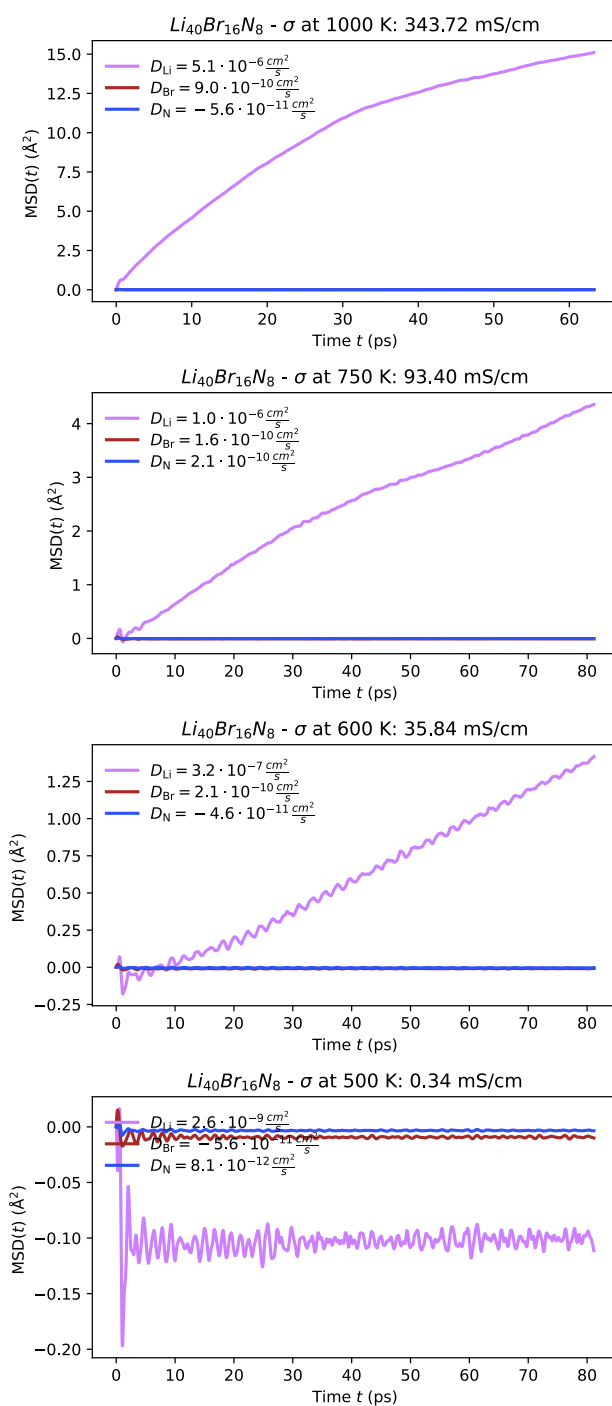


Fig. S27 MSD plot of Li along with host-lattice species of *Li₅Br₂N* at all temperatures studied with FPMD

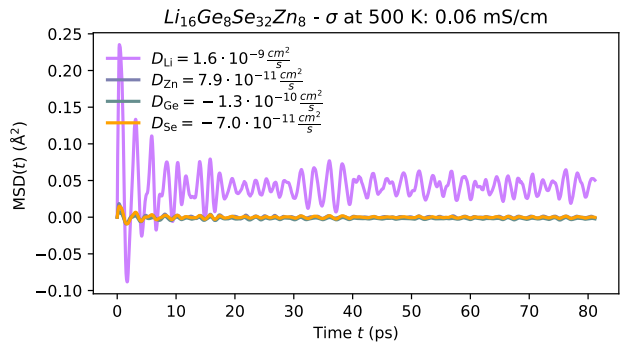
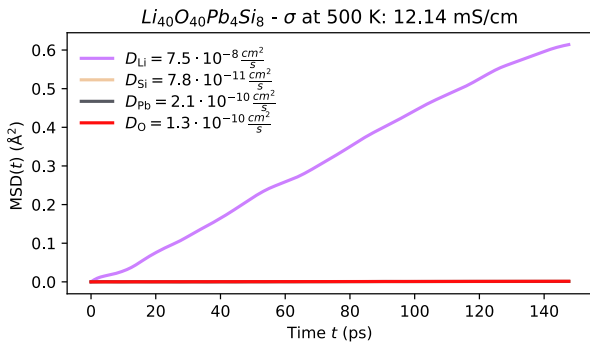
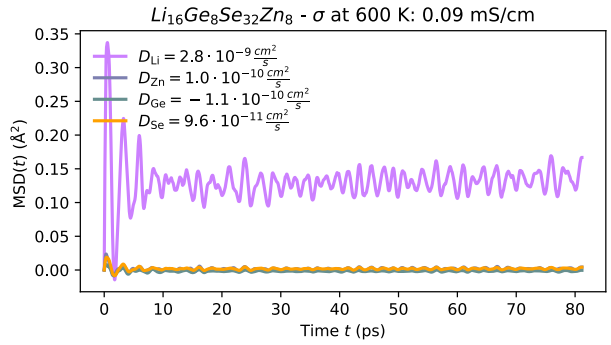
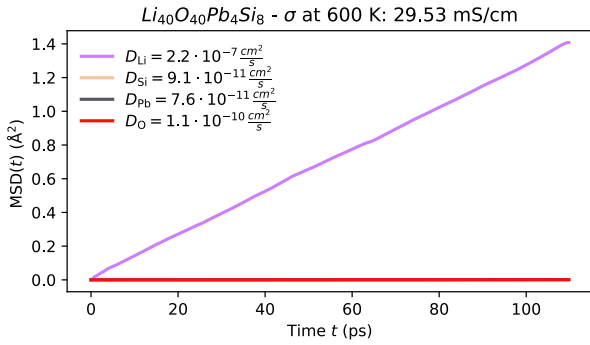
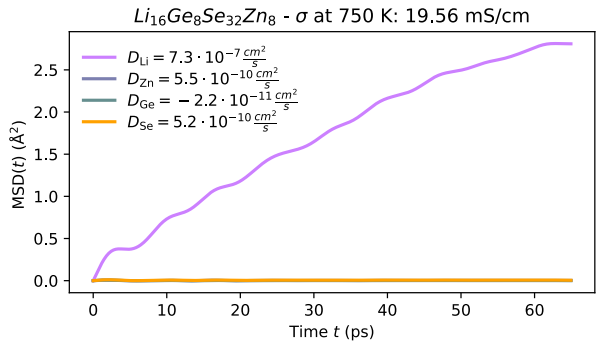
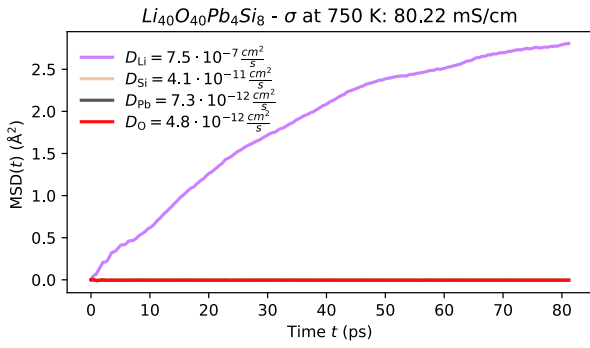
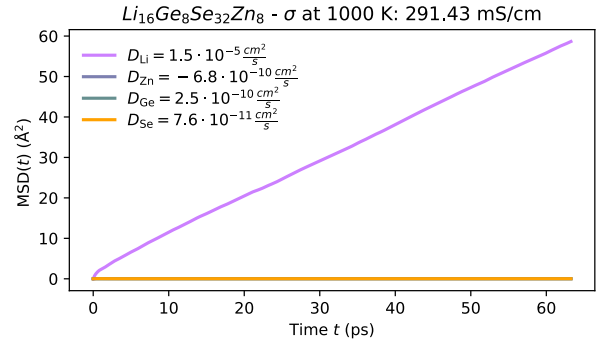
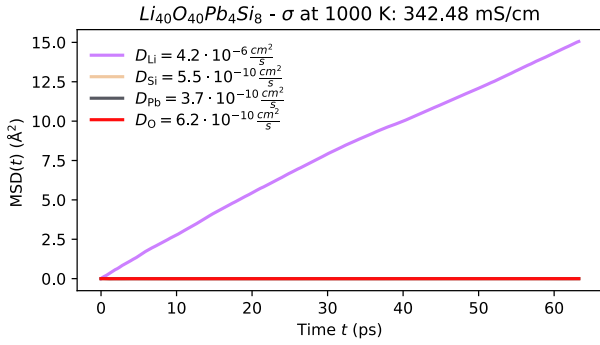


Fig. S28 MSD plot of Li along with host-lattice species of *Li₁₀Si₂PbO₁₀* at all temperatures studied with FPMD

Fig. S29 MSD plot of Li along with host-lattice species of *Li₂ZnGeSe₄* at all temperatures studied with FPMD

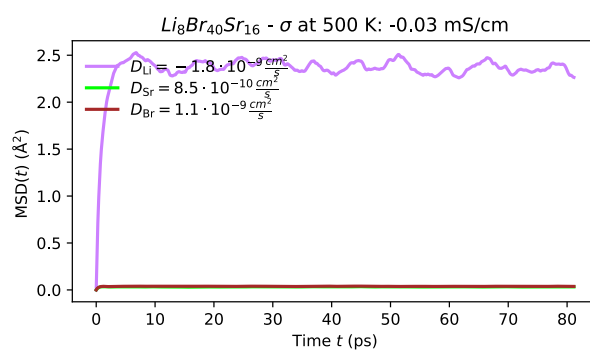
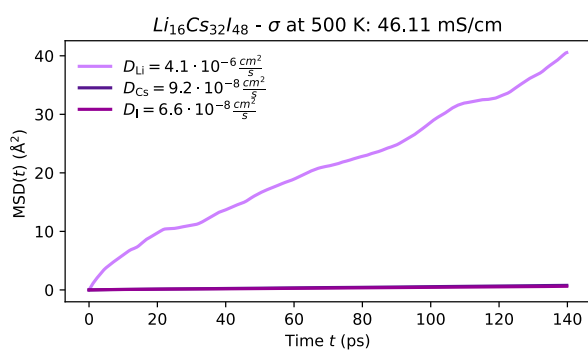
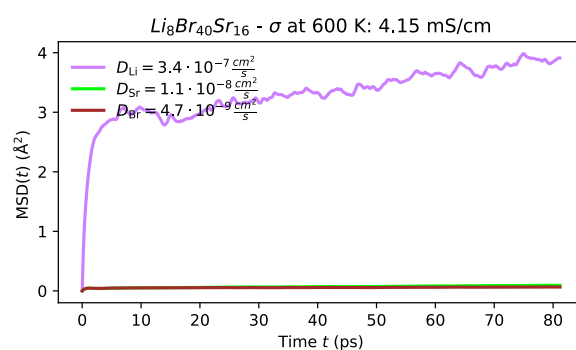
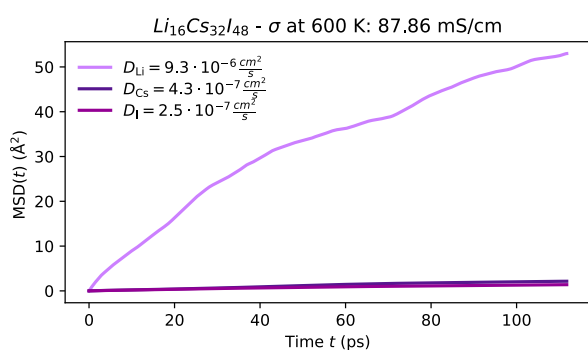
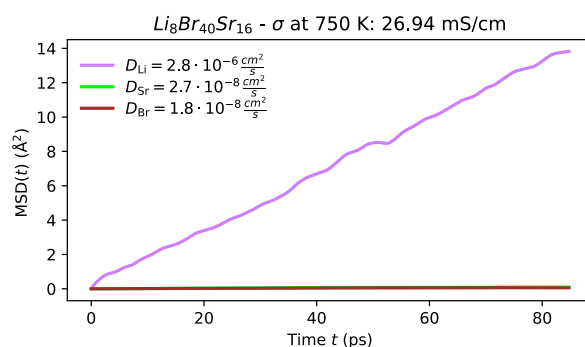
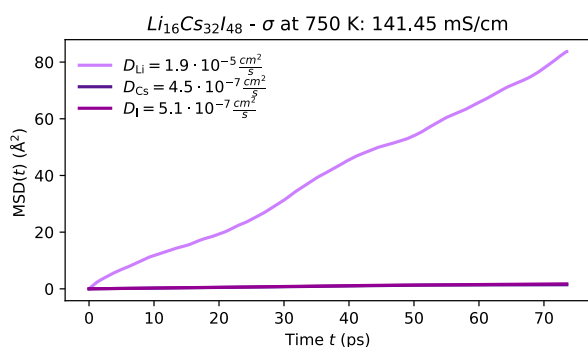
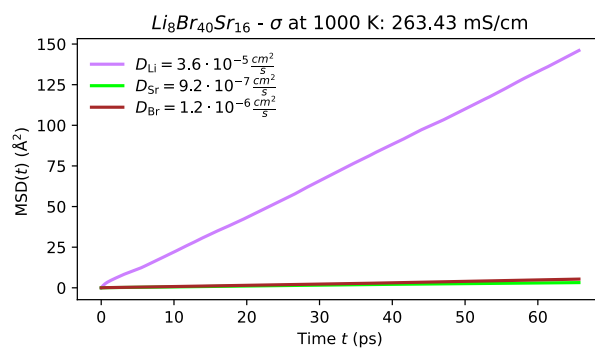
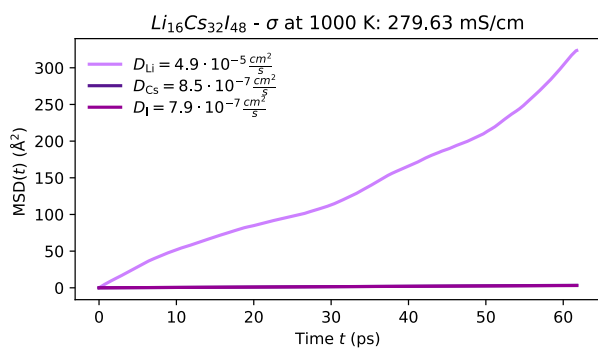


Fig. S30 MSD plot of Li along with host-lattice species of *LiCs₂I₃* at all temperatures studied with FPMD

Fig. S31 MSD plot of Li along with host-lattice species of *LiSr₂Br₅* at all temperatures studied with FPMD

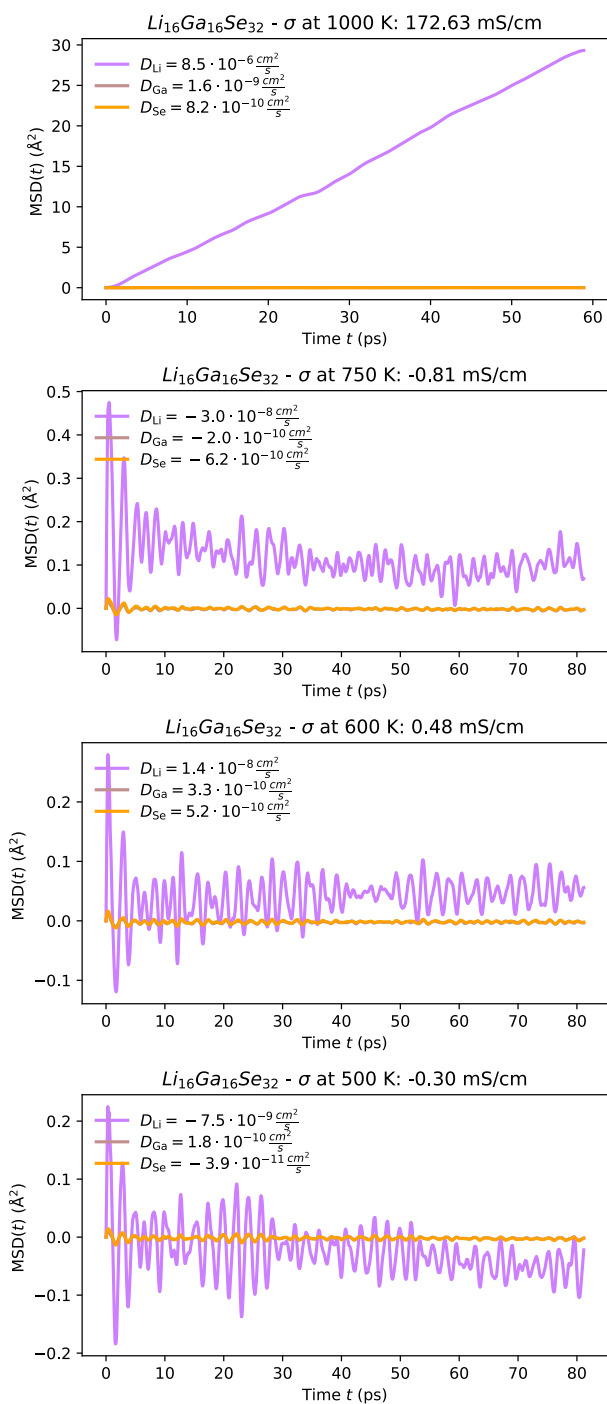


Fig. S32 MSD plot of Li along with host-lattice species of $LiGaSe_2$ at all temperatures studied with FPMD

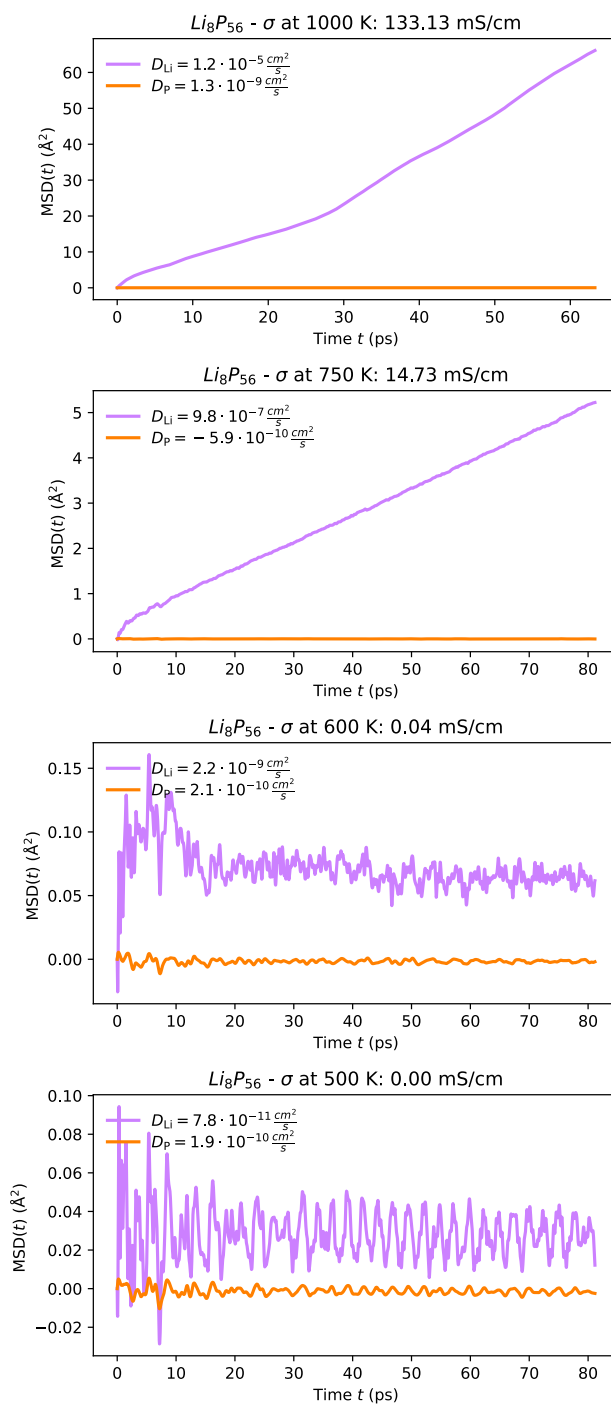


Fig. S33 MSD plot of Li along with host-lattice species of LiP_7 at all temperatures studied with FPMD

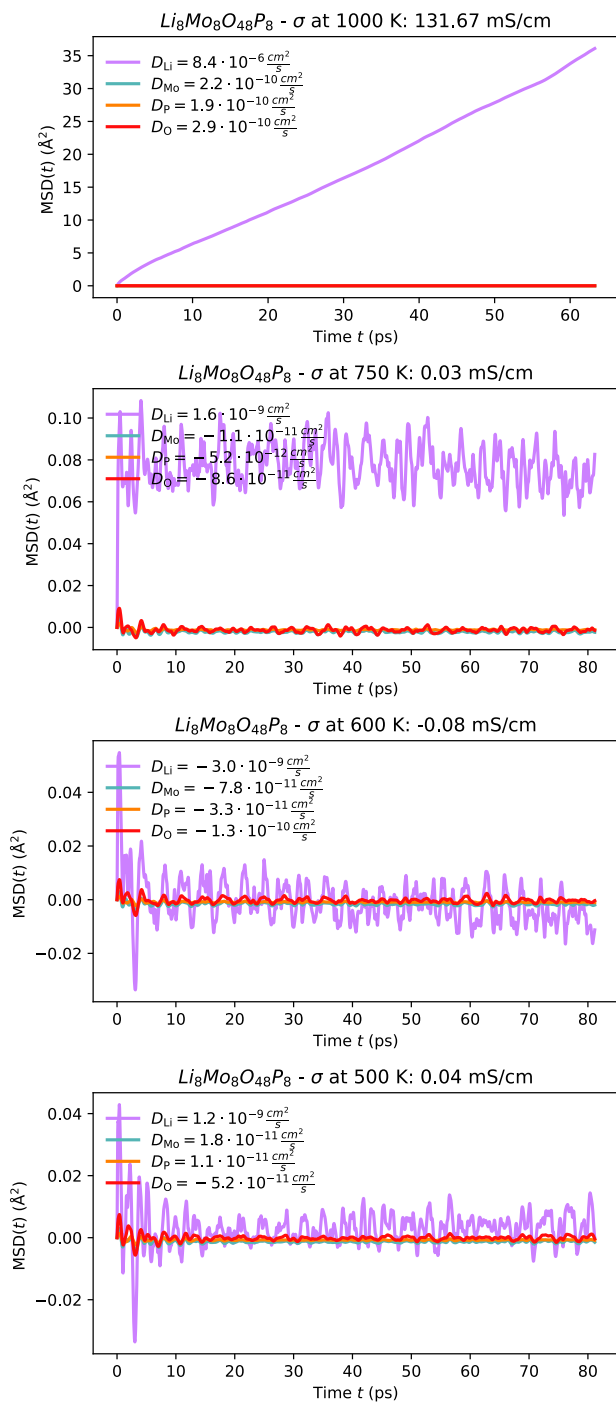


Fig. S34 MSD plot of Li along with host-lattice species of *LiMoPO₆* at all temperatures studied with FPMD

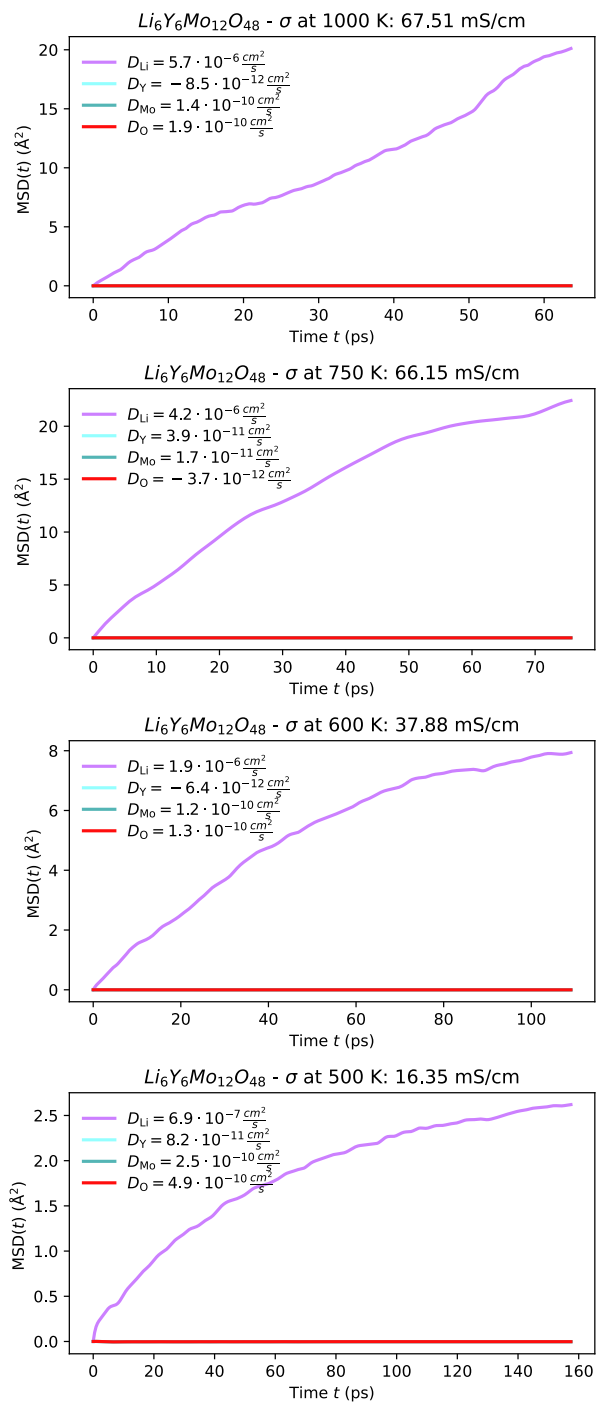


Fig. S35 MSD(t) plot of Li along with host-lattice species of *LiY(MoO₄)₂* at all temperatures studied with FPMD.

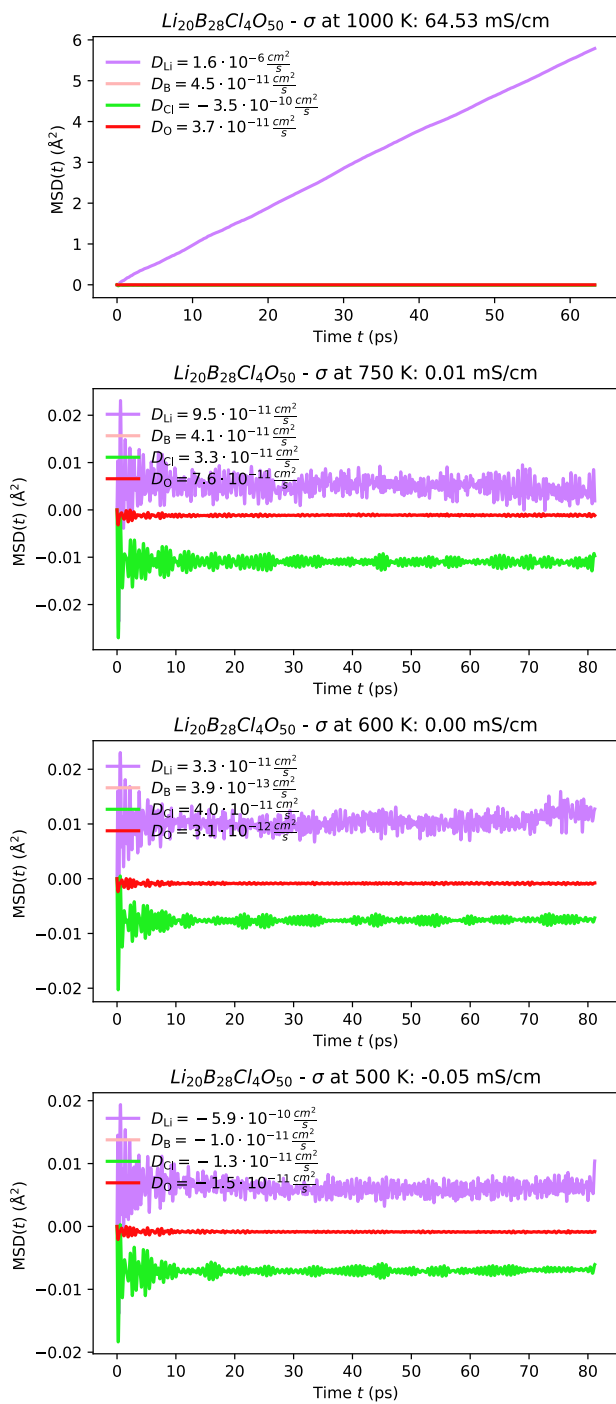


Fig. S36 MSD plot of Li along with host-lattice species of *Li₁₀B₁₄Cl₂O₂₅* at all temperatures studied with FPMD

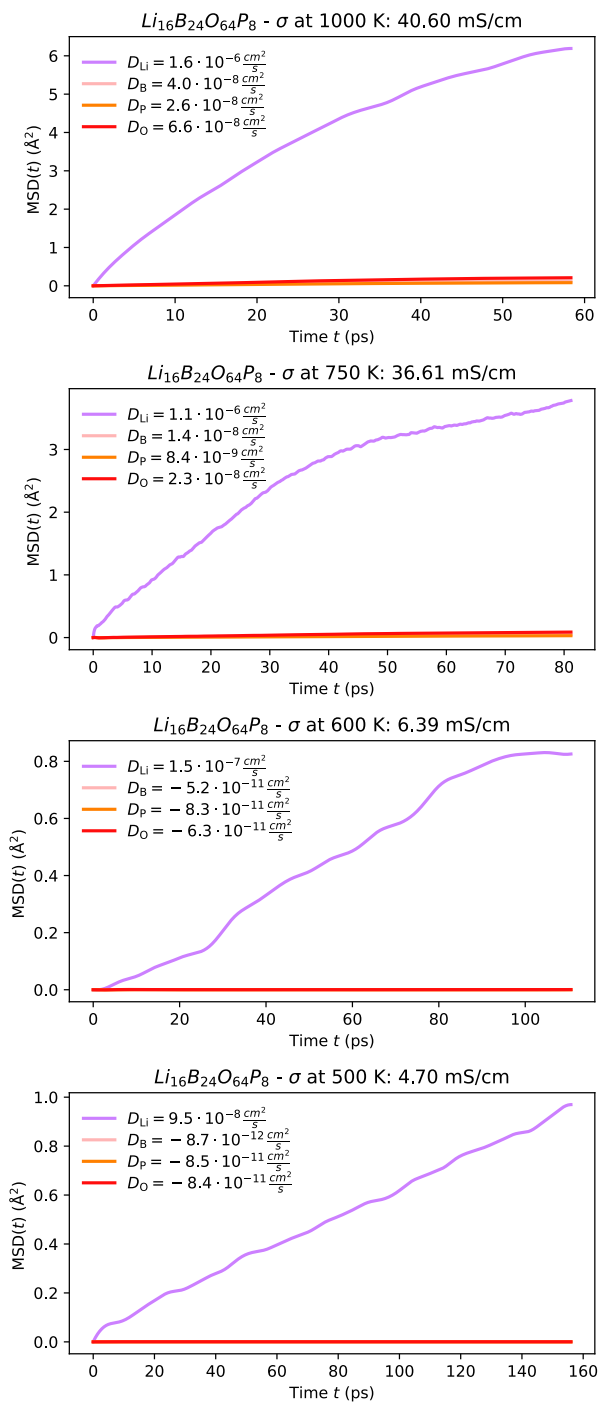


Fig. S37 MSD plot of Li along with host-lattice species of *Li₂B₃PO₈* at all temperatures studied with FPMD

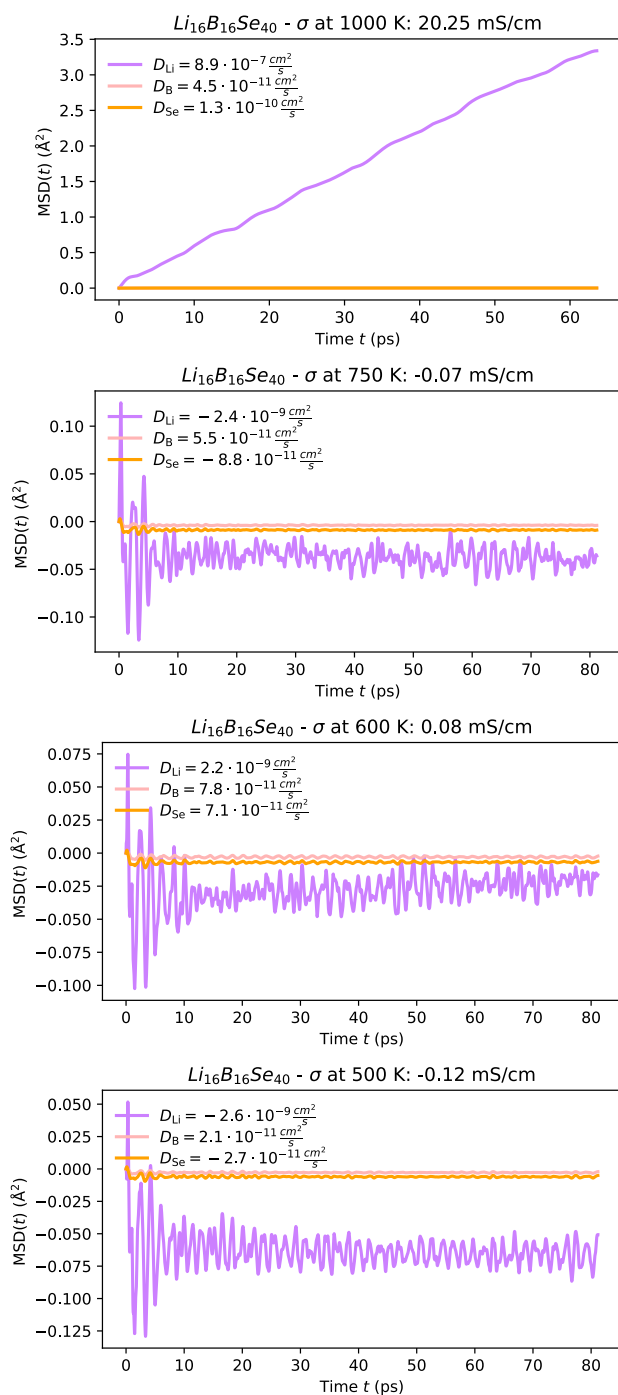


Fig. S38 MSD plot of Li along with host-lattice species of $\text{Li}_2\text{B}_2\text{Se}_5$ at all temperatures studied with FPMD

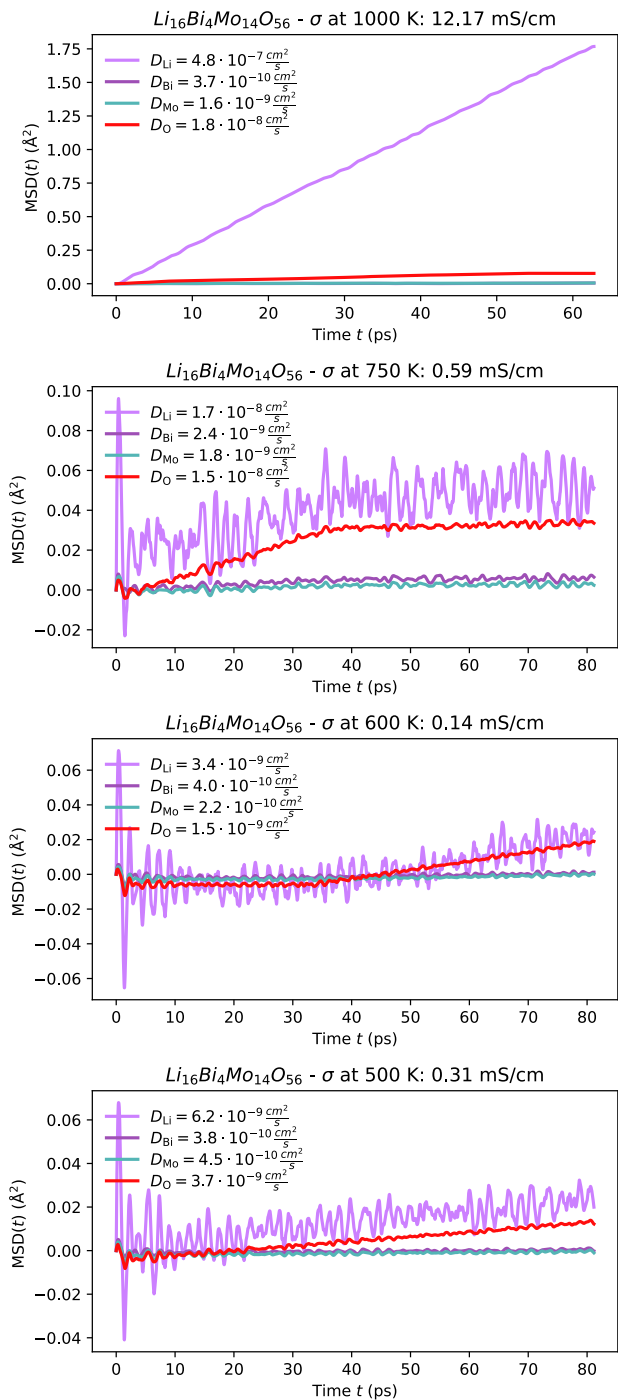


Fig. S39 MSD plot of Li along with host-lattice species of $\text{Li}_8\text{Bi}_2(\text{MoO}_4)_7$ at all temperatures studied with FPMD

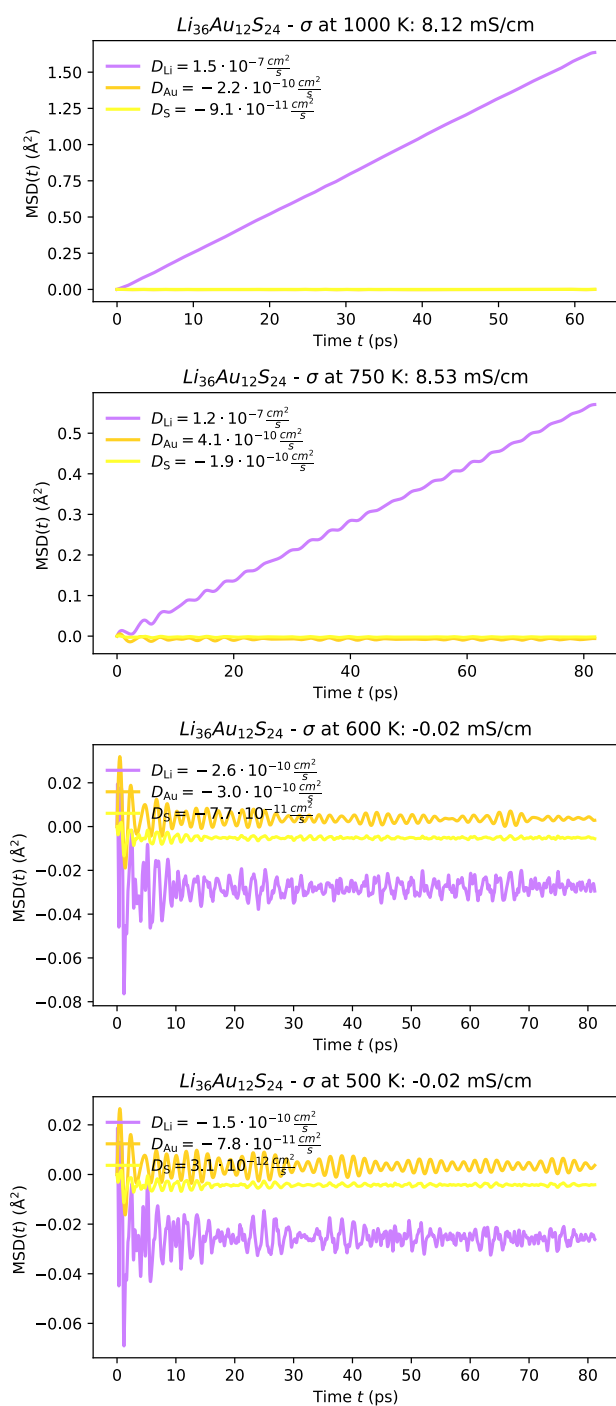


Fig. S40 MSD plot of Li along with host-lattice species of Li_3AuS_2 at all temperatures studied with FPMD

S3 Non diffusive structures

We find 18 materials that do not exhibit Li-ion diffusion in our FPMD simulations at 1000 K. We show the MSD plots only at 1000 K as we did not run FPMD at other temperatures on account of not being able to resolve diffusion at 1000 K.

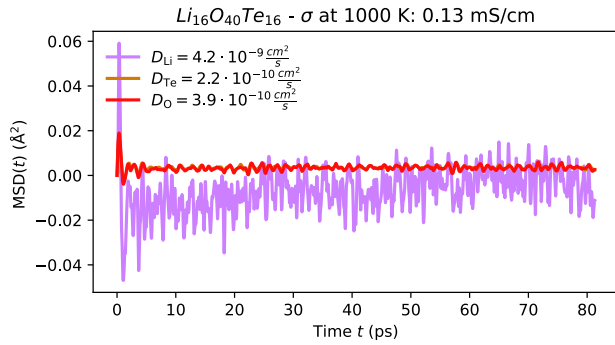


Fig. S41 MSD plot of Li along with host-lattice species of $Li_2Te_2O_5$ at 1000 K studied with FPMD

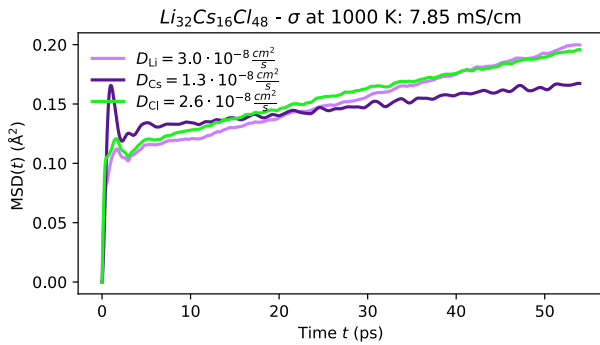


Fig. S42 MSD plot of Li along with host-lattice species of Li_2CsCl_3 at 1000 K studied with FPMD

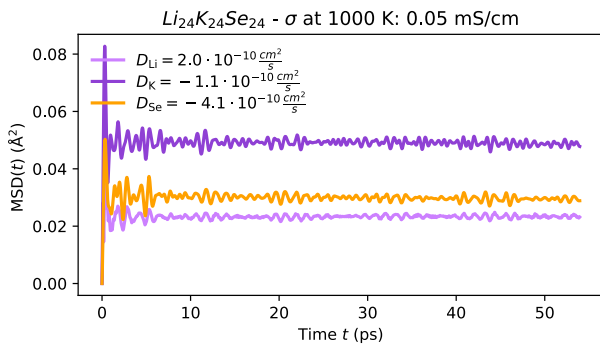


Fig. S43 MSD plot of Li along with host-lattice species of $LiKSe$ at 1000 K studied with FPMD

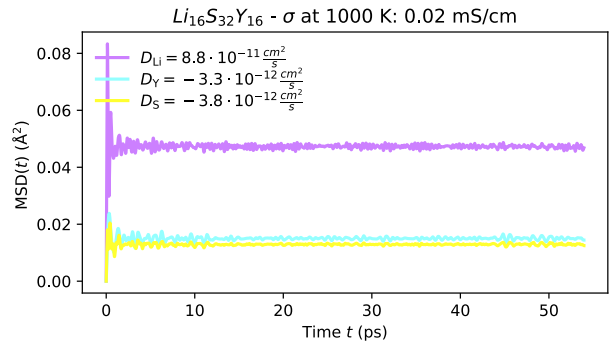


Fig. S44 MSD plot of Li along with host-lattice species of $LiYS_2$ at 1000 K studied with FPMD

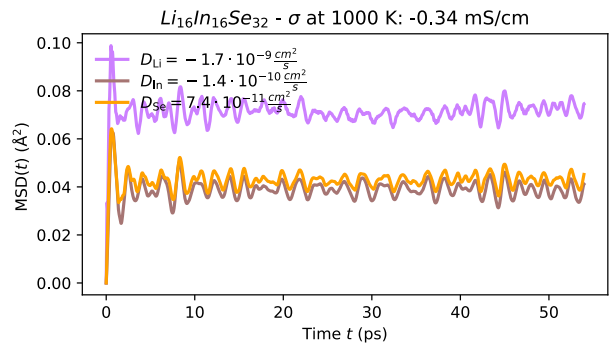


Fig. S45 MSD plot of Li along with host-lattice species of $LiInSe_2$ at 1000 K studied with FPMD

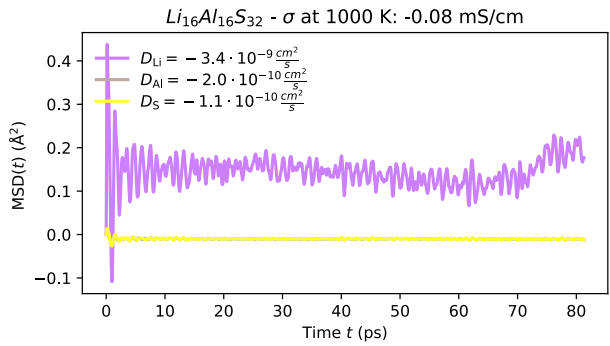


Fig. S46 MSD plot of Li along with host-lattice species of $LiAlS_2$ at 1000 K studied with FPMD

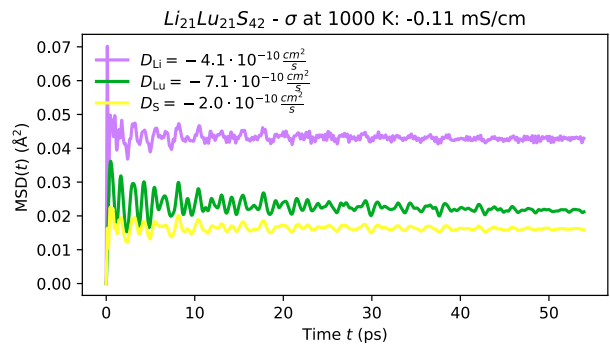


Fig. S47 MSD plot of Li along with host-lattice species of $LiLuS_2$ at 1000 K studied with FPMD

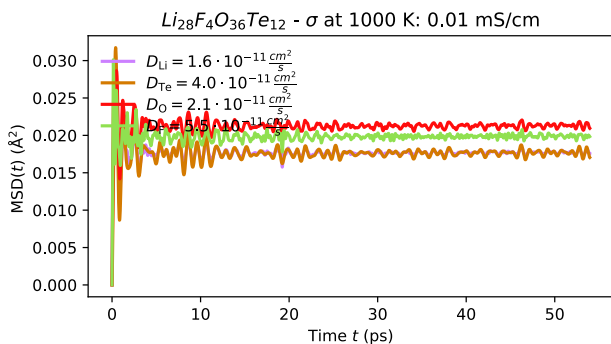


Fig. S48 MSD plot of Li along with host-lattice species of $Li_7Te_3O_9F$ at 1000 K studied with FPMD

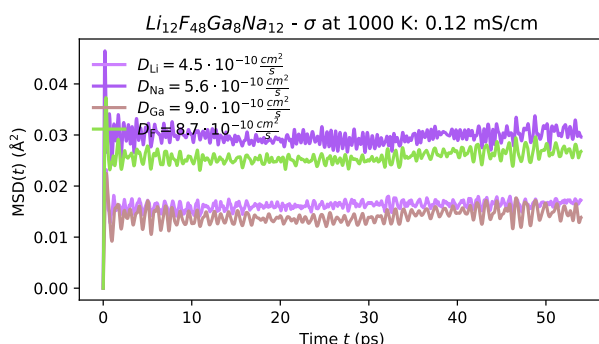


Fig. S52 MSD plot of Li along with host-lattice species of $Li_3Na_3Ga_2F_{12}$ at 1000 K studied with FPMD

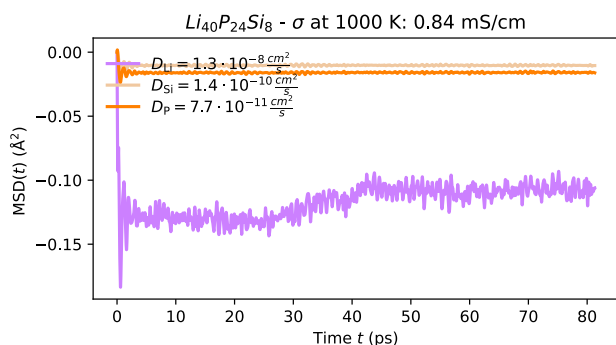


Fig. S49 MSD plot of Li along with host-lattice species of Li_5SiP_3 at 1000 K studied with FPMD

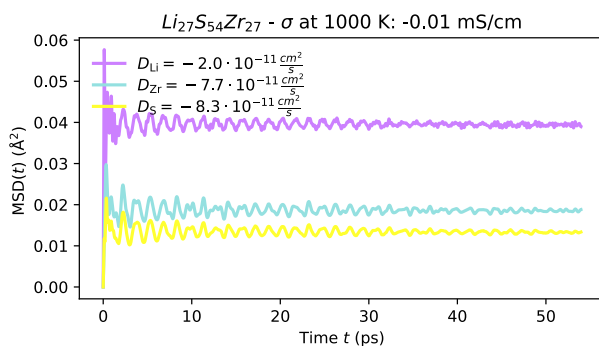


Fig. S53 MSD plot of Li along with host-lattice species of $LiZrS_2$ at 1000 K studied with FPMD

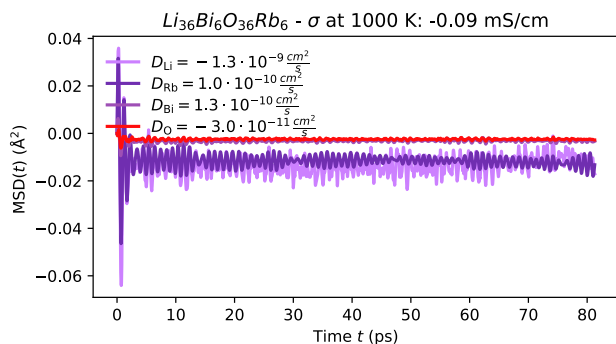


Fig. S50 MSD plot of Li along with host-lattice species of Li_6RbBiO_6 at 1000 K studied with FPMD

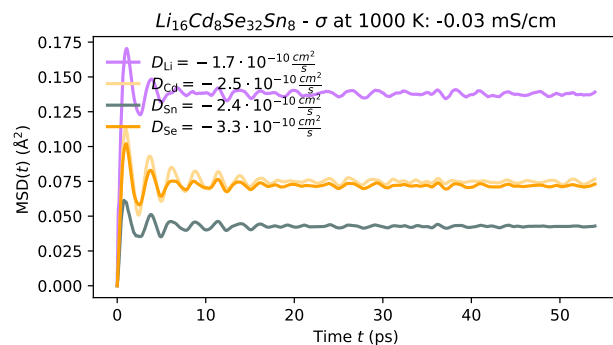


Fig. S54 MSD plot of Li along with host-lattice species of $Li_2CdSnSe_4$ at 1000 K studied with FPMD

Fig. 5

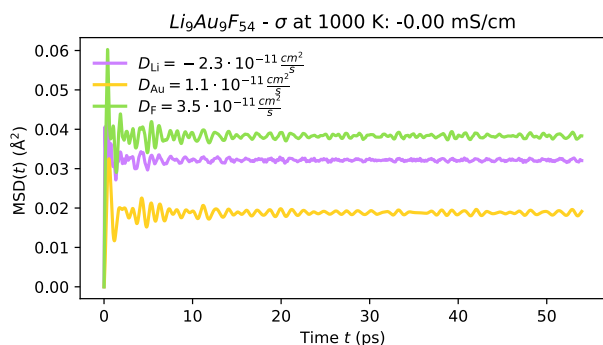


Fig. S51 MSD plot of Li along with host-lattice species of $LiAuF_6$ at 1000 K studied with FPMD

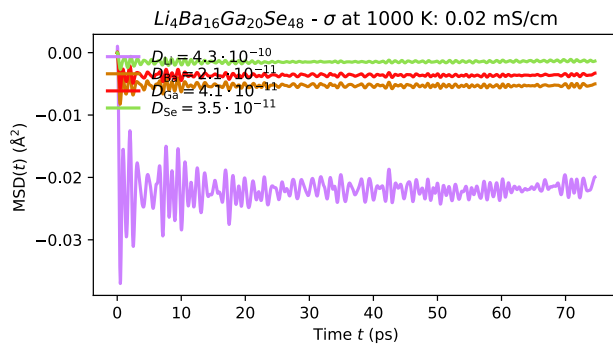


Fig. S55 MSD plot of Li along with host-lattice species of $LiBa_4Ga_5Se_{12}$ at 1000 K studied with FPMD

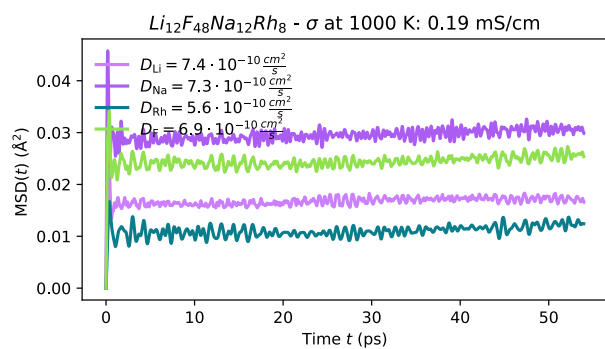


Fig. S56 MSD plot of Li along with host-lattice species of *Li₃Na₃Rh₂F₁₂* at 1000 K studied with FPMD

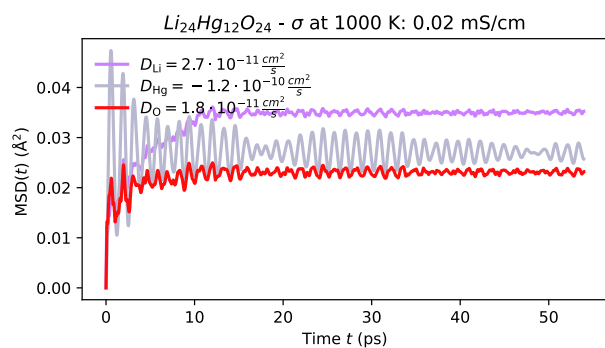


Fig. S57 MSD plot of Li along with host-lattice species of *Li₂HgO₂* at 1000 K studied with FPMD

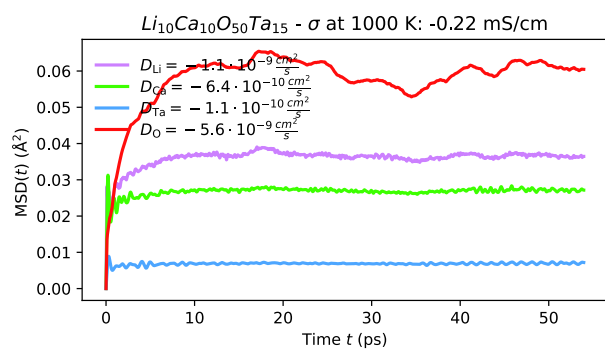


Fig. S58 MSD plot of Li along with host-lattice species of *Li₂Ca₂Ta₃O₁₀* at 1000 K studied with FPMD