

Supporting Information

Compositional transferability of deep potential in molten LiF-BeF₂ and LaF₃ mixtures: Prediction of density, viscosity, and local structure

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S1. RMSEs of energy and force

In **Fig. S1**, the energy and force of molten Flibe+LaF₃ achieve convergence after 1,000,000 training steps, and average RMSEs of the last 5000 training steps for energy and force are 1.9 meV atoms⁻¹ and 3.5×10^{-2} eV Å⁻¹, respectively.

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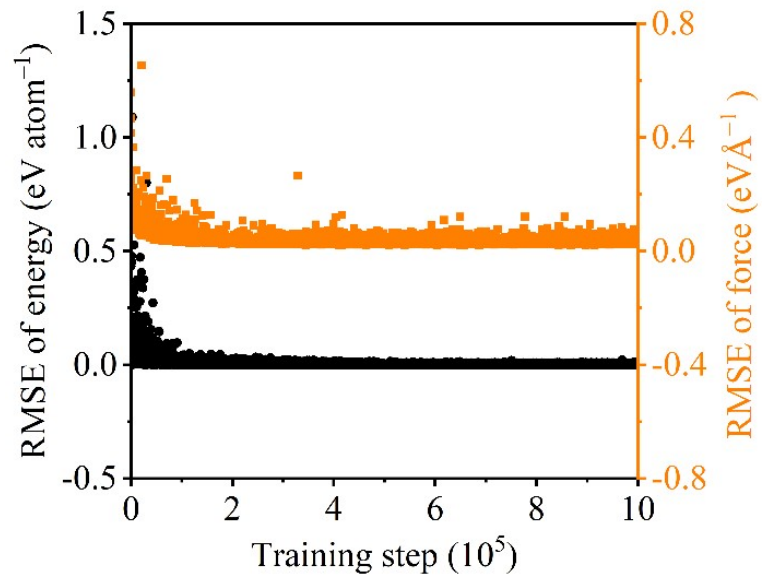


Fig. S1 RMSEs of energy (black points) and force (orange points) for molten Flibe+LaF₃ in the training stage

S2. DPMD simulated MSDs and RDFs

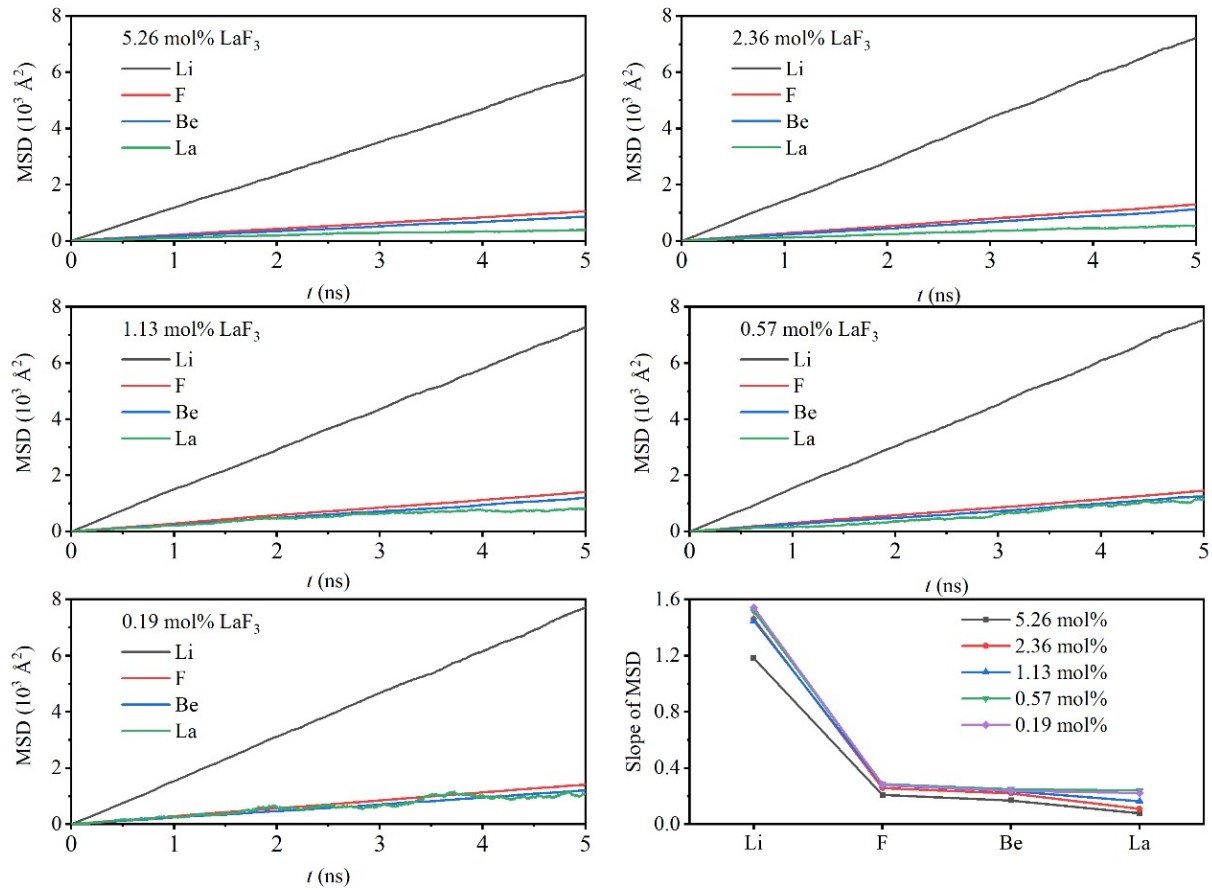


Fig. S2 MSDs of molten Flibe+LaF₃ at different LaF₃ concentrations and the slopes of MSDs

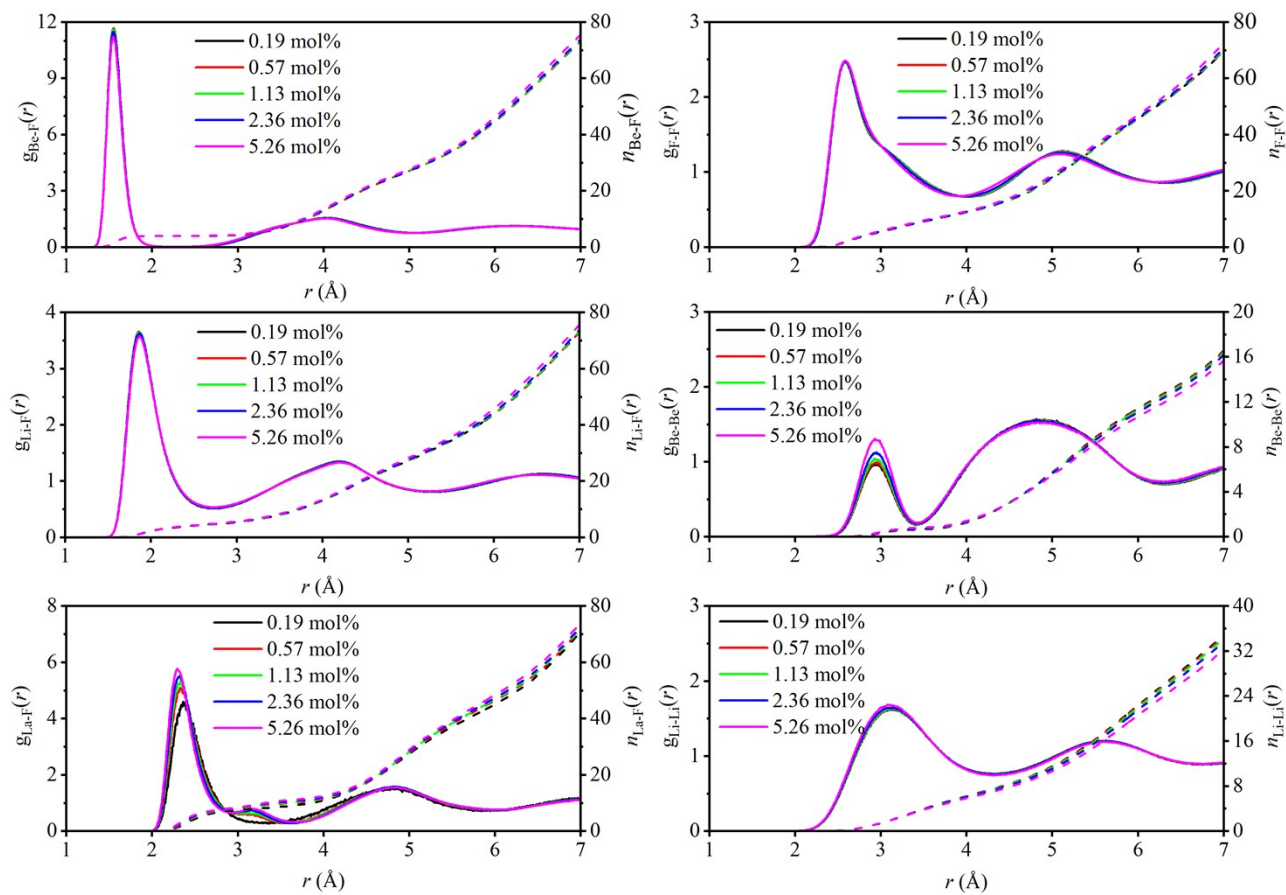


Fig. S3 RDFs and their integral curves of Be-F, Li-F, La-F, F-F, Be-Be, and Li-Li for molten

$\text{Flibe} + x\text{LaF}_3$