Supporting Information

Concentration–Transferable Deep Potential Molecular Dynamics: Unraveling Component–Structure–Transport in Molten $LiF–BeF_2–EuF_2$

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S1. RMSEs

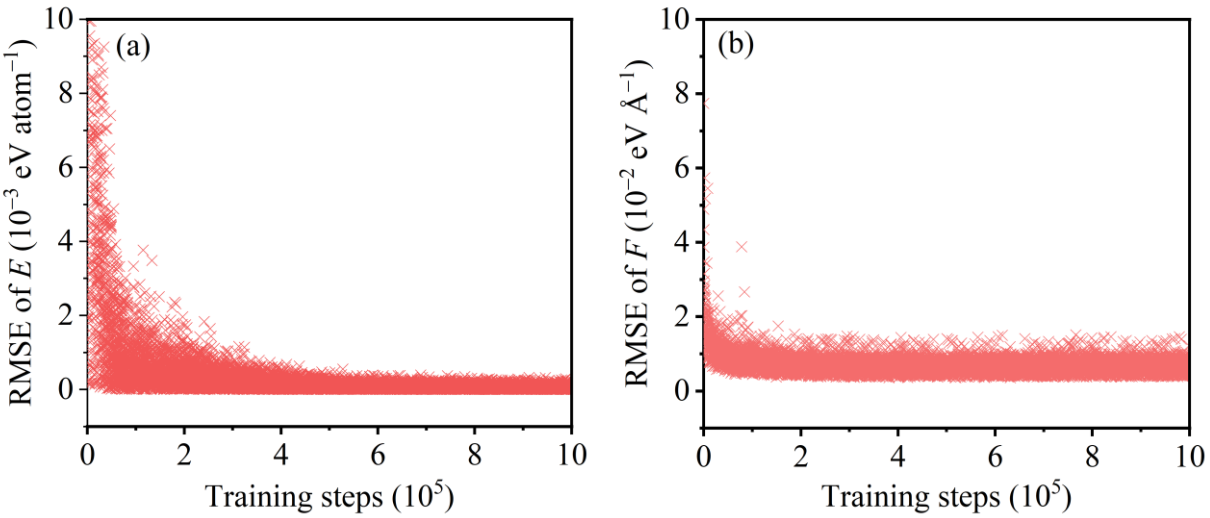

Figure S1 RMSEs of (a) energy and (b) force for molten FLiBeEu evaluated from training datasets

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S2. MSDs

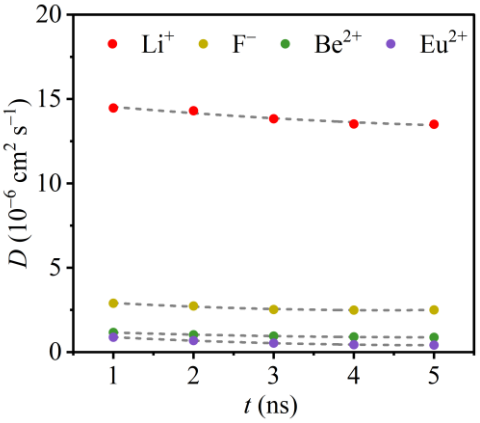

Figure S2 *D* variations with extended simulation duration for the S5 system (6.25 mol% EuF_2)

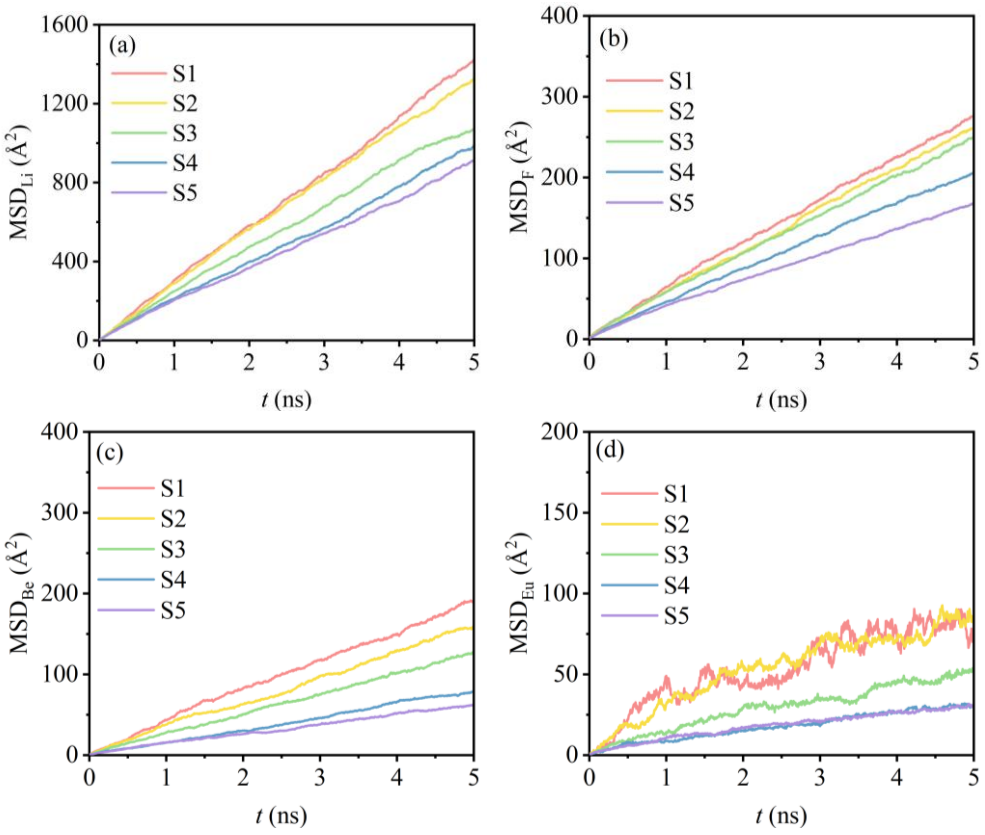

Figure S3 MSDs of (a) Li, (b) F, (c) Be, and (d) Eu ions in molten FLiBeEu with different EuF_2 concentrations at 823 K

S3. RDFs

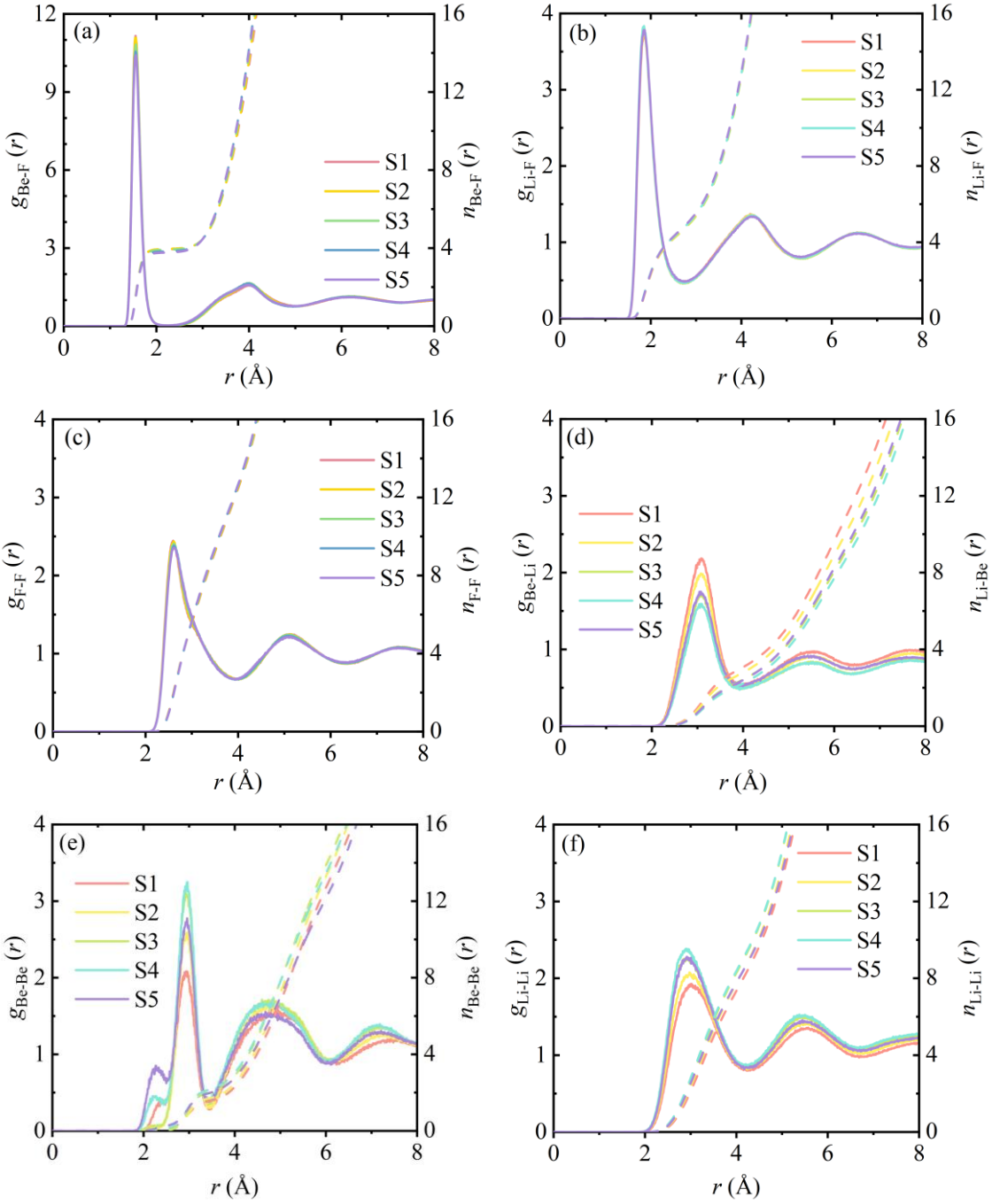

Figure S4 RDFs of (a) Be−F, (b) Li−F, (c) F−F, (d) Be−Li, (e) Be−Be, and (f) Li−Li ionic pairs for molten FLiBeEu with different EuF_2 concentrations at 823 K

Table S1 First-peak positions (R, Å) and heights (H) along with their relative deviations (ΔR= ($R_{DP}-R_{FP}$)/R_{FP} and ΔH= ($H_{DP}-H_{FP}$)/H_{FP}) for the RDFs of each ionic pair from FPMD, FPMD+U, and DPMD simulations at 6.25 mol% EuF_2

Ionic pair	R_{FP+U}	R_{FP}	R_{DP}	ΔR	H_{FP+U}	H_{FP}	H_{DP}	ΔH
Be−F	1.56	1.56	1.56	0	11.78	8.90	10.25	15.2%
Li−F	1.87	1.89	1.86	−1.6%	3.71	3.08	3.65	18.5%
F−F	2.57	2.62	2.64	0.8%	2.43	1.76	2.29	30.1%
Be−Be	2.92	2.94	2.94	0	1.14	0.78	3.01	285.9%
Be−Li	3.09	3.06	3.06	0	2.65	1.65	1.72	4.2%
Li−Li	3.11	3.04	2.94	−3.3%	1.81	1.91	2.21	15.7%
Eu−F	2.50	2.25	2.29	1.8%	3.71	4.11	5.27	28.2%
Eu−Be	3.35	2.94	2.80	−4.8%	2.60	1.78	2.74	53.9%
Eu−Eu	4.43	3.73	3.62	−2.9%	3.81	5.85	5.95	1.7%
Eu−Li	3.70	3.56	3.56	0	2.01	1.83	1.81	−1.1%

S4. Density of State (DOS)

To elucidate the driving forces of bond formation involving Eu in molten FLiBe, we performed electronic structure analysis on the final configuration obtained from AIMD simulations. Our results show that, a nonzero electron population emerges in the Eu 5d orbitals after equilibration, indicating charge transfer or orbital mixing with surrounding F ligands. However, a single static configuration cannot fully capture the detailed electronic structure of a molten salt; therefore, sampling multiple configurations along the simulation trajectory would yield greater statistical significance.

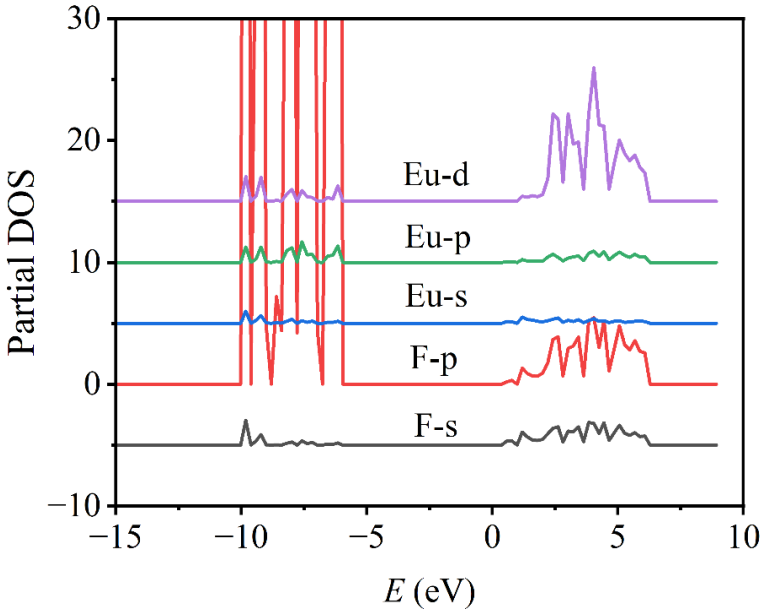

Figure S5 Partial DOSs of Eu and F in molten FLiBeEu with an EuF_2 concentrations of 6.25 mol%