

Comprehending the progressive structure of molten salt by deep potential molecular dynamics for high temperature heat storage

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Supplementary Information

Table S1. Local structural characteristics of ternary eutectic salt.

Parameters (Å)	<i>T</i> (K)	Na-Na	Na-K	Na-Cl	Na-O	K-K	K-Cl	K-O	Cl-Cl	C-O	O-O
<i>r</i> _{max}	873K	3.737	4.075	2.702	2.314	4.389	3.099	2.722	4.090	1.308	2.267
	923K	3.751	4.078	2.702	2.312	4.390	3.096	2.722	4.112	1.308	2.267
	973K	3.759	4.089	2.698	2.311	4.391	3.094	2.715	4.122	1.308	2.267
	1023K	3.792	4.115	2.694	2.310	4.409	3.087	2.715	4.132	1.308	2.267
	1073K	3.823	4.139	2.693	2.309	4.430	3.084	2.718	4.166	1.308	2.267
<i>r</i> _{min}	873K	6.525	6.775	4.275	3.375	5.625	4.575	3.675	6.375	1.730	2.675
	923K	6.475	6.725	4.125	3.325	5.575	4.625	3.725	6.375	1.780	2.675
	973K	6.425	6.725	4.175	3.375	5.725	4.675	3.775	6.425	1.730	2.675
	1023K	6.525	6.725	4.225	3.375	5.825	4.775	3.825	6.425	1.780	2.675
	1073K	6.525	6.925	4.175	3.325	5.825	4.775	3.825	6.425	1.780	2.675
<i>r</i> _{avg}	873K	5.864	2.580	3.398	2.322	4.102	4.782	2.179	10.860	3.000	2.000

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923K	5.864	2.580	3.398	2.322	4.102	4.782	2.179	10.860	3.000	2.000
973K	5.804	2.563	3.395	2.296	4.053	4.738	2.198	10.853	3.000	2.000
1023K	5.642	2.492	3.340	2.256	3.930	4.640	2.165	10.627	3.000	2.000
1073K	5.519	2.410	3.278	2.224	3.858	4.566	2.109	10.425	3.000	2.000

Transport properties

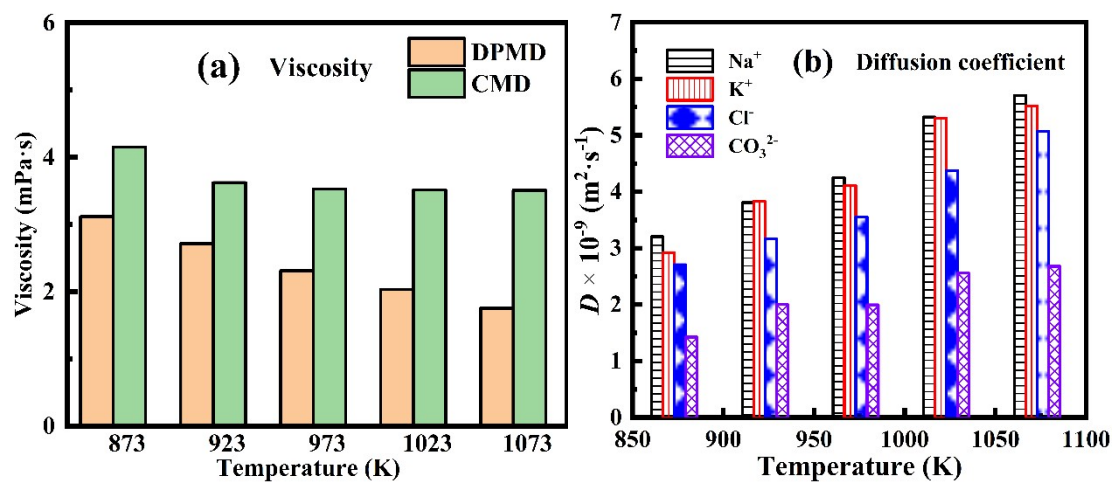


Figure S1. (a) Viscosity and (b) diffusion coefficient.