Supporting Information for "Mechanism Exploration of the Enhancement of Thermal Energy Storage in Molten Salt nanofluid"

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The Born-Mayer-Huggins (BMH) potential with Coulomb potential, shown in Eq. (S1), was used to describe the interaction between two no-bonded atoms of the carbonate base fluid[1]. Meanwhile, the bonded interactions with bond stretching, bond bending and torsion in CO_3^{2-} were calculated as Eq. (S2)[2]. Besides, the Buckingham potential with Coulombic interaction, shown in Eq. (S3)[3], was used to describe the interaction between two non-bond atoms in the SiO_2 nanoparticle. The Lennard-Jones (L-J) with Coulombic interaction, shown in Eq. (S4), was applied as force field for the Al_2O_3 nanoparticle. The bonded interactions with bond stretching, bond bending and torsion is shown in Eq. (S2)[4]. For both two nanofluid, the interaction between nanoparticle and base fluid was described by L-J potential energy with Coulombic interaction, shown in Eq. (S4). Moreover, the Particle-particle-particle-mesh (pppm) with an accuracy of 10^{-4} was used for coulombic interactions in the MD simulation of this paper[5]. The parameters used in the potential mentioned above are all given in the Table S1.

$$E_{ij}(r) = \frac{z_i z_j e^2}{r_{ij}} + \mathrm{b}(1 + \frac{z_i}{n_i} + \frac{z_j}{n_j}) \exp[\alpha(\sigma_i + \sigma_j - r_{ij})] \quad \text{(S1)}$$

where z_i and z_j are the ion valences of ion i and j, e is the electric charge unit, n_i and n_j are the number of electrons in the outer atomic shell, σ_i and σ_j, can be interpreted as the ionic radius and r_{ij} is the distance between atoms i and j. Moreover, the constants b=4.865 kcal/mol and σ=3.45 $Å^{-1}$ determine the weight and steepness of the BMH interaction[1], respectively.

$$E_{\mathrm{bond}} = \mathrm{K_s}(r - r_0)^2 + \mathrm{K_b}(\theta - \theta_0) + \mathrm{K_t}(1 + d \cdot \cos(n\phi)) \quad \text{(S2)}$$

where K_s, K_b and K_t are the stretching constant, bending constant and torsional constant, respectively. Besides, r and θ are the bond length and bond angle, r_0 and θ_0 are the bond length and angle at a balanced condition.

$$E_{ij}(r) = A_{ij} e^{-\frac{r_{ij}}{\rho_{ij}}} - \frac{C_{ij}}{r_{ij}^{6}} + \frac{q_i q_j}{r_{ij}} \quad \text{(S3)}$$

where E_{ij} is the interaction energy, r_{ij} is the distance between site i and j. q_i and q_j are the charges of the atom at site i and j, respectively.

$$E_{ij}(r) = \frac{q_i q_j}{r_{ij}} + 4\xi[(\frac{\sigma_{ij}}{r_{ij}})^{12} - (\frac{\sigma_{ij}}{r_{ij}})^{6}] \quad \text{(S4)}$$

where r_{ij} is the distance between atom i and j, and ξ_{ij} is the potential well depth while σ_{ij} is the distance between atom i and j where the inter-particle potential is zero.

Table S1 (a). Potential parameters for the carbonate base fluid in this study[2, 6]

Parameters		Carbonate salt base fluid				
BMH potential		Interaction	C-C	O-O	K-K	Li-Li
		q (e)	1.54	-1.18	1.00	1.00
		n	2.46	7.18	8.00	2.00
		σ (Å)	1.10	1.33	1.39	0.77
Bonded interactions	Stretching	K_s (Kcal/mol/Å^2)	4612			
		r_o (Å)	1.29			
	Bending	K_b (Kcal/mol)	107.435			
		θ_0 (°)	120			
	Torsion	K_t (Kcal/mol)	1.139			
		d	-1			
		n	0			

Table S1 (b). Potential parameters for the SiO_2 nanoparticle in this study[3]

Atom	q_i (e)	A_{ii} (Kcal·mol^{-1})	ρ_{ii} (Å)	C_{ii} (Kcal·mol^{-1}·Å^6)
O (In SiO_2)	-0.955209	15170.70	0.386	617.24
Si	1.910418	72460.64	0.351	14415.29

Table S1 (c). Potential parameters for the Al_2O_3 nanoparticle in this study[4]

Parameters		Al_2O_3 nanoparticle			
L-J potential	Interaction	Al-Al		O-O	
	ξ (Kcal/mol)	0.040		0.228	
	σ (Å)	4.053		2.860	
	q (e)	1.5		-1.0	
Bonded interactions	Stretching	K_s (Kcal/mol/Å^2)		392.8	
		r_o (Å)		1.775	
	Bending	K_b (Kcal/mol)	100.3	K_b (Kcal/mol)	31.1
		θ_0 (°)	109.5	θ_0 (°)	149.8
	Torsion	K_t (Kcal/mol)		26.270	
		d		-1	
		n		2	

Table S1 (d) L-J potential parameters for the interaction between nanoparticle and base fluid[4, 6, 7]

Materials	Interaction	ξ (Kcal/mol)	σ(Å)	q (e)
SiO_2	Si-Si	0.040	4.053	1.910418
	O-O(in SiO_2)	0.228	2.860	-0.955209
Al2O3	Al-Al	0.040	4.053	1.5
	O-O(in Al_2O_3)	0.228	2.860	-1.0
	C-C	0.148	3.617	1.54
Carbonate base fluid	O-O(in CO_3^{2-})	0.228	2.88	-1.18
	K-K	5.451	3.197	1
	Li-Li	4.735	2.839	1

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