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1 **Effect of Al₂O₃ nanoparticle dispersion on the specific heat**
2 **capacity of a eutectic binary nitrate salt for solar power**
3 **applications**

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11 **Abstract:** Molten salts can be used as heat transfer fluids or thermal storage materials
12 in a concentrated solar power plant. Improving the thermal properties can influence the
13 utilization efficiency of solar energy. In this study, the effect of doping eutectic binary
14 salt solvent with Al₂O₃ nanoparticles on its specific heat capacity (c_p) was investigated.
15 The effects of the mass fraction of nanoparticles on the c_p of the composite nanofluid
16 were analyzed, using both differential scanning calorimetry measurements and
17 molecular dynamics simulations. The specific heat capacity of the nanocomposites
18 was enhanced by increasing the nanoparticle concentration. The maximum
19 enhancement was found to be 8.3%, at a nanoparticle concentration of 2.0%. A
20 scanning electron microscope was used to analyze the material morphology. It was
21 observed that special nanostructures were formed and the specific heat capacity of the
22 nanocomposites was enhanced by increasing the quantity of nanostructures.
23 Simulation results of c_p agreed well with the experimental data, and the potential
24 energy and interaction energy in the system were analyzed. The change in Coulombic
25 energy contributed to most of the large change in c_p , which explains the discrepancy
26 in values between conventional nanofluids and molten salt-based nanofluids.

27 **Keywords:** solar energy application; nanocomposite; specific heat capacity;
28 molecular dynamics simulation; potential energy analysis

29
30

31 **1. Introduction**

32 The depletion of fossil fuels and the harmful gas emissions during the burning of
33 fossil fuels compel the search for renewable and clean energy sources and higher
34 efficiency of energy utilization [1–3]. To solve the energy crisis, some researchers
35 focus on improving heat transfer efficiency via optimizing the heat transfer surface
36 [4–7] while others tend to using high performance working media [8,9]. Meanwhile,
37 the development of renewable energy was investigated. Solar energy is regarded as
38 the best potential source to replace fossil fuels, with the average amount of energy
39 transported to the earth as sunlight in one hour able to provide all of the energy
40 currently consumed globally in one year [10]. A promising technology for the
41 collection and use of solar energy is the concentrating solar power (CSP) system,
42 which transforms solar energy to thermal energy with a heat-transfer fluid (HTF) [11].
43 Mahian et al.[12,13] used different working fluids in solar collectors and investigated
44 the thermal efficiency. In solar collectors, lower specific heat capacity will induce a
45 higher outlet temperature, increasing the solar energy utilization efficiency. However,
46 solar energy is quite unsteady and unpredictable, since it varies from day to night, by
47 cloud condition, and season. Hence, a working medium is needed to store the energy
48 when it is available and then release it when there is insufficient sunlight. Considering
49 the large amount of HTF and thermal energy storage (TES) materials required in a
50 CSP plant, it is necessary to reduce the cost of these materials while improving their
51 heat transfer and thermal storage performance. With thermal stability, comparable
52 viscosity, and low vapor pressure at high temperature, various molten salts are used in
53 modern CSP systems [14]. Solar salt, with a composition of 60% NaNO_3 and 40%
54 KNO_3 by weight, was used in the Solar Two central receiver systems [15] and other
55 solar plants [16]. Other molten salts are also being researched to improving the
56 thermal performance [17–19].

57 However, these molten salts also have some disadvantages that limit the
58 applicability of solar plants, for instance relatively low specific heat capacity and
59 thermal conductivity [20]. Doping base fluids with nanosized particles to make
60 nanofluids [21] is a potential way to improve their thermal properties, especially
61 thermal conductivity [22]. Wen et al. [23] reviewed the heat transfer applications of
62 nanofluids, including their formulations, influences on the effective thermal
63 conductivity, and enhancement mechanisms. In previous research, various mechanisms
64 have been identified that could enhance the effective thermal conductivities of these

65 materials, including the formulation of an interfacial layer, Brownian motion of the
66 nanoparticles, ballistic transport of energy carriers, and structural effects. Most of the
67 research has focused on thermal conductivity; however, the influence of nanoparticles
68 on the specific heat capacity is still unclear [24].

69 Das et al. [25,26] investigated the specific heat capacity of nanofluids using a
70 mixture of water and ethylene glycol as the base fluid. Silica, zinc oxide, and alumina
71 nanoparticles were used and results indicated that the c_p decreased with an increase in
72 the nanoparticle concentration, but increased with increasing temperature. Similar
73 results were found by Zhou et al. [27] with CuO nanofluids, Zhou and Ni [28] with
74 Al_2O_3 nanofluids, and Elias et al. [29] with Al_2O_3 nanofluids. It seems that for
75 conventional nanofluids (those with water, oil, ethylene glycol, or alcohol as the base
76 fluid), the specific heat capacity is reduced by doping with nanoparticles. However,
77 with molten salt or an ionic liquid as the base fluid, the influence of adding
78 nanoparticles had the opposite effect. He et al. [30] prepared a carbonate salt/carbon
79 nanomaterial composite to enhance the performance of a high-temperature salt. Both
80 the specific heat capacity and thermal conductivity were significantly enhanced. Ding
81 et al. [31] prepared a mixture of solar salt and nanoparticles by mechanic grinding and
82 mixing. An enhancement of 10.48% in the specific heat capacity was obtained by
83 adding CuO nanoparticles up to a mass concentration of 0.1%. Beyond this
84 concentration, however, the enhancement worsened, and the specific heat capacity
85 deteriorated at a concentration of 1.5%. Ho and Pan [32] formulated the Hitec-based
86 Al_2O_3 nanocomposite in a specially designed rid at high temperature. They studied the
87 effects of nanoparticle concentration on the specific heat capacities of nanocomposites
88 and found that the optimal concentration was 0.063% with an enhancement of 20%.
89 Jo and Banerjee [33,34] investigated the influence of graphite and multi-walled
90 carbon nanotubes (MCNT) on the specific heat capacity of a carbonate mixed salt. An
91 enhancement greater than 20% was obtained, and molecular dynamics simulations
92 (MDS) were carried out to better understand the tremendous improvement. Shin et al.
93 [35–39] performed a series investigation on carbonate salt-based SiO_2
94 nanocomposites. The enhancement in the specific heat capacity varied from 5% to
95 30%, and they proposed three models to explain the enhancement: (1) a higher c_p for
96 the silica nanoparticles than that of the bulk material; (2) solid-fluid interaction energy;
97 and (3) a semi-solid layer formulation of liquid molecules surrounding the
98 nanoparticles. Lu et al. [40] and Schuller et al. [41] prepared solar salt-based Al_2O_3
99 nanocomposites using a similar method, but obtained contrary results. The former

100 showed a decrease in the c_p , while in the latter it was enhanced 30.6%.

101 Though several studies have reported increased specific heat capacity, the rules
102 and mechanisms involved for this increase in molten salts with nanoparticle doping
103 are still insufficient. Most explanations about the significant enhancement of c_p were
104 based on some assumptions. In the present work, different mass fractions of solar
105 salt-based nanofluids were investigated using experimental measurements and
106 simulations. The nanomaterials were prepared by a dissolution method, and the specific
107 heat capacity was measured by a differential scanning calorimeter (DSC) using the
108 sapphire method. Material morphology analysis was conducted by a scanning electron
109 microscope. The effects of nanoparticles on the potential energy were then analyzed
110 by molecular dynamics simulations.

111 **2. Experiment**

112 **2.1 Nanocomposite synthesis**

113 In this study, we used the liquid solution method proposed by Shin et al. [36] to
114 formulate the nanocomposites. Sodium nitrate and potassium nitrate were procured
115 from Tianjin Fengchuan Chemical Reagent Technologies Co., Ltd., both with purities
116 above 99.0%. Al_2O_3 nanoparticles were purchased from Beijing Dk Nanotechnology
117 Co. Ltd. The average diameter was about 20 nm and the purity was 99.99%. The
118 procedure followed for obtaining the molten salt nanomaterial is illustrated in figure 1.
119 Initially, 5 mg of Al_2O_3 nanoparticles were added to 20 mL of deionized water, which
120 was then stirred for 20 min to form a suspension. Then, the suspension was sonicated
121 for 60 min in an ultrasonicator (PS-100A, Jieken Ultrasonic Cleaner Limited, China) at
122 a frequency of 40 kHz to ensure good dispersion and to minimize the potential
123 agglomeration of nanoparticles. After that, different weights of the solar salt were
124 dissolved in the suspension, so that the mass fraction of nanoparticles varied from 0.5%
125 to 2.0%. The mixture was ultrasonicated for another 60 min to guarantee uniformity of
126 the mixture. After sonication, the solution was then heated in a vacuum drying oven at
127 atmospheric pressure with a temperature setting of 110 °C, according to the research
128 of Jo [34] that evaporation temperature has little effect on the results. It was heated for
129 7 hours to obtain the dehydrated salt, which was the testing material for the DSC. All
130 powders were weighed using an electronic microbalance (Sartorius MC 21S). It should
131 be noted that there is no dispersing agent used in the preparation procedure.

132 **2.2 Measurement of specific heat capacity**

133 The specific heat capacities of the samples were measured based on the sapphire
134 method using a DSC (204F1, NETZSCH). Aluminum pans were used to contain the
135 samples, and the sample masses ranged from 5 mg to 15 mg. To protect the instrument
136 from potential damage, the aluminum pans were covered with pierced lids. In the
137 sapphire method, the heat flow through an empty pan, an aluminum pan with sapphire,
138 and an aluminum pan with a prepared sample is measured. Then, using the three results
139 and the specific heat capacity of sapphire, the specific heat capacity of each sample is
140 calculated. The samples were heated to 50 °C and maintained at this temperature for 5
141 min to stabilize the calorimeter signal. A ramping rate of 20 °C/min was then applied,
142 with the end temperature set to 450 °C. The sample was maintained at 450 °C for 5 min
143 to ensure signal stability. Each sample was measured 3 times following the same
144 procedure.

145 **2.3 Uncertainty analysis**

146 Uncertainties in the experimental results are dependent on the measurement
147 deviations for each of the parameters, including mass and heat flow. The specific heat
148 capacity was determined by Equation (1):

$$149 \quad c_{p,s} = c_{p,sapp} \cdot \frac{\Delta q_s \cdot m_{sapp}}{\Delta q_{sapp} \cdot m_s} \quad (1)$$

150 where c_p is the specific heat capacity, q is the heat flow, m is the weight, and the
151 subscripts s and sapp denote sample and sapphire. Taking f as a function of several
152 independent parameters f_i , and each uncertainty as Δf_i , then the uncertainty of the
153 experiment can be expressed as:

$$154 \quad d(\ln f) = \sum_{i=1}^n \left| \frac{\partial \ln f}{\partial f_i} \right| \Delta f_i \quad (2)$$

155 The accuracy of the electronic balance was ± 0.005 mg, and the accuracy of the heat
156 flow measurement was ± 0.1 μ W. Hence, the maximum measurement uncertainty of
157 the specific heat capacity was estimated to be 2.4%.

158

159 3. Molecular dynamics simulations

160 Molecular dynamics (MD) simulations were performed to explore interactions
161 between the nanoparticles and solvent molecules using the Large-scale
162 Atomic/Molecular Massively Parallel Simulator (LAMMPS) package. Initially, one
163 Al₂O₃ nanoparticle fixed with a diameter of 2 nm was placed in the center of the
164 simulation box and the solar salt molecules were placed randomly in the box, as
165 shown in figure 2. The length of the simulation box was varied to adjust the
166 nanoparticle mass concentration from 0% to 2.0%.

167 The Lennard-Jones (L-J) potential with long-range Coulombic force was
168 employed to calculate the interaction between two non-bonded atoms, as shown in
169 Equation (3), where $E(r)$ is the potential of the two atoms, r is their distance from each
170 other, q_i and q_j are the charges on atoms i and j , respectively, ϵ is the potential well depth,
171 and σ is the finite distance at which the inter-particle potential is zero. The L-J
172 parameters between different atomic species were calculated by the Berthlot mixing
173 rule [42], as shown in Equation (4). In addition, bond stretching, bond bending, and
174 torsion were considered for the bonded interactions, as shown in Equation (5), where r
175 is bond length, θ is bond angle, ϕ is torsional angle, k_s , k_b , k_t are stretching, bending
176 and torsional constants, respectively. All parameters used for the different atoms in the
177 MD simulation are listed in Table 1.

$$178 \quad E(r) = \frac{q_i q_j}{r} + 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad (3)$$

$$179 \quad \epsilon_{i,j} = \sqrt{\epsilon_i \cdot \epsilon_j}, \quad \sigma_{i,j} = \frac{(\sigma_i + \sigma_j)}{2} \quad (4)$$

$$180 \quad E = k_s \cdot (r - r_0)^2 + k_b \cdot (\theta - \theta_0) + k_t \cdot (1 + d \cdot \cos(n\phi)) \quad (5)$$

181 Since the solar salt molecules were randomly placed in the simulation box, it is
182 highly possible that there would be overlapping atoms, which would result in
183 non-physical interactions. Hence, an energy minimization step was implemented to
184 redistribute the atoms. During this step, the temperature of the system was reduced to
185 zero K. Afterwards, a microcanonical ensemble was used to perform the relaxation
186 procedure. Subsequently, the system temperature was raised to 650 K. A canonical
187 Nose-Hoover thermostat (NVT integration, with a constant number of atoms N ,
188 volume of the system V , and temperature T controlled through direct temperature
189 scaling) was used for the temperature range from 650 to 800 K to obtain the specific

190 heat capacity of the system.

191 **4. Results and Discussion**

192 **4.1 Specific heat capacity results**

193 The solar salt was doped with Al₂O₃ nanoparticles with an average diameter of 20
194 nm at mass fractions of 0.5%, 1.0%, 1.5%, and 2.0%. To guarantee the accuracy of the
195 instrument, the melting temperature and enthalpy of Sn and Bi were measured and
196 good agreement was shown with reference values, as shown in table 2.

197 Figure 3 shows the variations in the specific heat capacities of the base salt and
198 nanocomposite mixtures in the full temperature range (80 °C to 400 °C). There are two
199 peaks in the temperature range, at about 130 °C and 227 °C, which indicate the phase
200 change temperatures. The peak at about 130 °C was formed by the solid-solid phase
201 change of the eutectic salt and the peak at about 227 °C was formed by the solid-liquid
202 phase change, agreeing with data from the literature [43] in which the respective peaks
203 were at 130.4 °C and 224.8 °C. The specific heat capacity of the base salt in the liquid
204 phase had an average value of 1.56 J/(g·K), showing a good agreement with values in
205 the literature of 1.50 to 1.53 J/(g·K) [44], a less than 5% error. It also can be seen that
206 the specific heat capacities of the samples changed only slightly with temperature,
207 indicating that temperature does not substantially affect the specific heat capacities of
208 these samples. In other words, the specific heat capacity is nearly independent of
209 temperature. Meanwhile, we can see that with an increase in the mass fraction of the
210 Al₂O₃ nanoparticles, the specific heat capacity of the samples increased.

211 Thermal energy storage (TES) capacity is an important parameter for TES systems,
212 since it influences the scope of the system and the operating cost. The TES capacity (Q)
213 was calculated as below.

$$214 \quad Q = \frac{\int_{260^{\circ}\text{C}}^{400^{\circ}\text{C}} h(T) dT}{m dT / dt} \quad (6)$$

215 where h is the heat flow, T is the working temperature, m is the weight of the sample,
216 and dT/dt is the heating rate. The total Q for pure base salt and after adding 0.5, 1.0, 1.5,
217 and 2.0 wt.% nanoparticles were 219.03, 223.01, 231.07, 233.84, and 236.32 kJ/kg in
218 the working temperature range of 260–400 °C, respectively. This indicates that the Q
219 value of the nanocomposite with ~2.0 wt.% nanoparticles has a maximum increase of
220 17.29 kJ/kg. Figure 4 plots Q versus temperature for pure base salt and after adding

221 different amounts of nanoparticles. With increasing the nanoparticle mass fraction, the
222 TES capacity increases in the working temperature range of 260–400 °C.

223 Usually, the specific heat capacity of the mixture is calculated using a simple
224 mixing model. The mixing model is based on the assumption of thermal equilibrium
225 between the particles and fluid and can be expressed as:

$$226 \quad c_{p,nf} = \frac{m_{np}c_{p,np} + m_s c_{p,s}}{m_{nf}} \quad (7)$$

227 where c_p is the specific heat capacity, m is the mass, and the subscripts nf , np , and s
228 denote the property values of the nanofluid, nanoparticle, and salt, respectively. The
229 specific heat capacity of the base salt and Al_2O_3 particles are 1.56 J/(g·K) and 1.12
230 J/(g·K), respectively, as measured in present work. Figure 5 shows a comparison
231 between the experimental value and the value predicted by the simple mixing model.
232 The measured average specific heat capacity of the base salt and nanocomposites,
233 from lowest to highest concentration, were 1.56 J/(g·K), 1.59 J/(g·K), 1.65 J/(g·K),
234 1.67 J/(g·K), and 1.69 J/(g·K), respectively. This indicates that the specific heat
235 capacity of the nanocomposite with an Al_2O_3 particle concentration of about 2.0% by
236 weight has a maximum enhancement of about 8.3%. However, the prediction values
237 decreased with an increase in the nanoparticle mass fraction, indicating that the
238 simple mixing model is not applicable in the evaluation of the specific heat capacity
239 of a nanocomposite.

240 4.2 Material Characterization

241 Since the specific heat capacity has a close relationship with the phase or
242 structure of the material, scanning electron microscope (SEM) (Quanta 200FEG) was
243 used to perform material characterization analyses. Figure 6 shows an SEM image of
244 the salt with various concentrations of nanoparticles after the DSC measurement. The
245 surface of the base salt was relatively smooth and had few visible structures. With the
246 addition of nanoparticles, some punctate and nubby microstructures appear (Figure 6
247 a). Adding more nanoparticles (Figure 6 b, c, and d) increases the quantity of these
248 microstructures and decreases the structure size. This kind of microstructure results in
249 an increase of the surface area. Due to the mismatch of vibrational density of states
250 between liquid and solid phase, there will be an interfacial thermal resistance, well
251 known as Kapitza resistance [45]. With the increase of the surface area, the total
252 interfacial thermal resistance will increase significantly [46,47], which will provide
253 additional thermal storage being responsible for enhancing the specific heat capacity.

254 4.3 Molecular dynamics simulations

255 To verify the accuracy of the MD simulations, the densities and c_p values of the
256 solar salt mixed with different mass concentrations of nanoparticles were calculated.
257 Figure 7 shows the comparison of density results from the MD simulation system and
258 theoretical calculation using Equation (8). Good agreement was obtained.

$$259 \quad \rho_{nf} = \varphi \rho_p + (1 - \varphi) \rho_f \quad (8)$$

260 where φ is the volume fraction of nanoparticles and the subscripts p and f denote the
261 nanoparticles and fluid, respectively.

262 In figure 8, it can be seen that the total energy of the ensemble changes linearly
263 with temperature for various nanoparticle mass concentrations, with an Adj. $R^2 >$
264 0.998. Hence, the c_p of the solar salt-based nanofluid is almost constant in the
265 temperature range of 650-800 K.

266 The specific heat capacity, c_p , is calculated as:

$$267 \quad c_p = \frac{\Delta E}{\Delta T \cdot V \cdot \rho} \quad (9)$$

268 where ΔE is the energy change, ΔT is the temperature change, V is the volume, and ρ is
269 the density of the ensemble. Figure 9 shows the experimental and simulated c_p values
270 with different nanoparticle mass concentrations. Acceptable agreement was
271 obtained—for pure base salt, c_p obtained from the MD simulation was 1.491 J/(g·K)
272 with an error of about -4.42% compared with the experimental value of 1.56 J/(g·K).
273 The same trend with nanoparticle concentration was also obtained: c_p increased with
274 increasing nanoparticle mass concentration, and at 2.0 wt.% nanoparticles, the c_p
275 enhancements were 6.24% and 8.33%, respectively, for the simulation and
276 experiment.

277 In order to explain this unusual enhancement of the c_p , we analyzed the energy
278 components and interaction for each atomic type (figure 10) in the simulation. The
279 energy of each atom can be divided into two parts: the kinetic energy (E_{ke}) and the
280 potential energy (E_{pe}), as shown in Equation (10).

$$281 \quad E = E_{ke} + E_{pe} \quad (10)$$

282 where the potential energy is composed of Van der Waals energy (E_{vdw}), Coulombic
283 energy (E_{coul}), long-range k-space energy (E_{long}), and molecular energy (E_{mol}). From
284 Figure 10, we can see that there was no significant change for E_{ke} , E_{vdw} , and E_{long} ,
285 while E_{pe} increased with the nanoparticle mass concentration due to the increase of

286 E_{coul} and E_{mol} . In other words, adding nanoparticles does not change the movement of
287 molecules, the interaction potential between two atoms and the energy in k space.
288 Figure 10 (b) shows the energy of three different intermolecular interactions in NO_3^- .
289 All of them change only slightly, indicating that the influence of added nanoparticles
290 on the molecular structure of NO_3^- is negligible. Hence, the slight increase in E_{mol} per
291 atom is due to the high molecular energy of Al_2O_3 . Only the Coulombic energy
292 change significantly for different nanoparticle mass fractions. Hence, the
293 enhancement of c_p is mainly due to the increase of the Coulombic energy, which can
294 also explain the different effects on c_p from adding nanoparticles to conventional base
295 fluids and molten salts. Since there are more ions in molten salt, the influence of the
296 Coulombic force is more significant.

297 **Conclusion**

298 In this study, the specific heat capacities of a binary nitrate salt and
299 nanocomposites with different mass fractions of added nanoparticles (0, 0.5, 1.0, 1.5,
300 and 2.0 wt.%, respectively) were investigated. The nanocomposites were synthesized
301 using a solution method. DSC was employed to measure the specific heat capacity.
302 Results show that the enhancement of the specific heat capacity of nanocomposites
303 ranges from 1.9% to 8.3% with an increase in the mass fraction of added
304 nanoparticles. The simple mixing model failed to predict the specific heat capacity of
305 the molten salt-based nanofluids. Material characterization analyses were carried out
306 using SEM. From the SEM images, we can see the formulation of punctate or nubby
307 nanostructures, which may induce the enhancement of specific heat capacity through
308 the enlarged specific surface area. The influence of nanoparticles on the energy
309 components of each atomic type was analyzed by molecular dynamics simulations.
310 Results indicate that the change in Coulombic energy per atom contributes the
311 greatest portion of the enhanced c_p .

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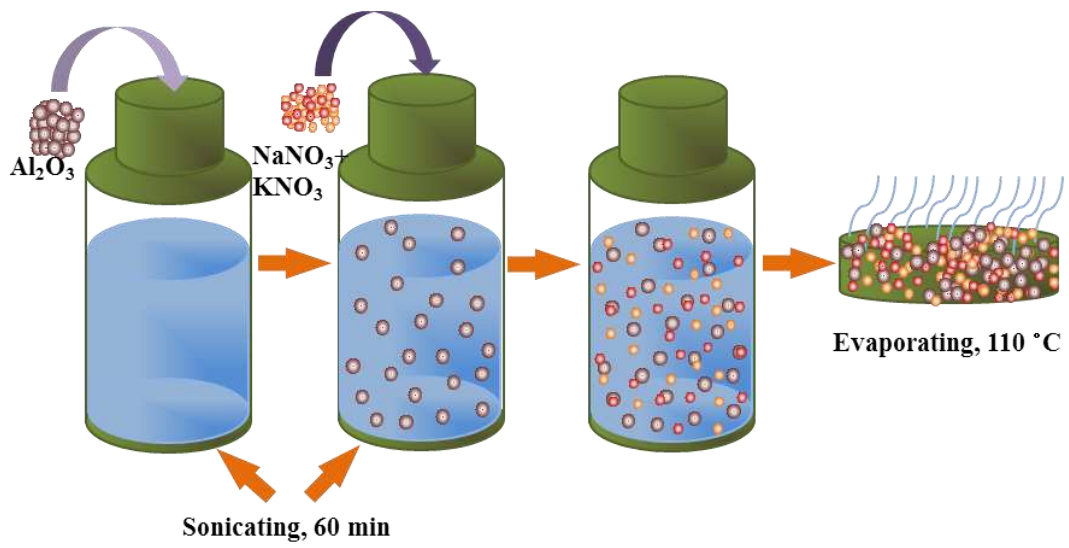
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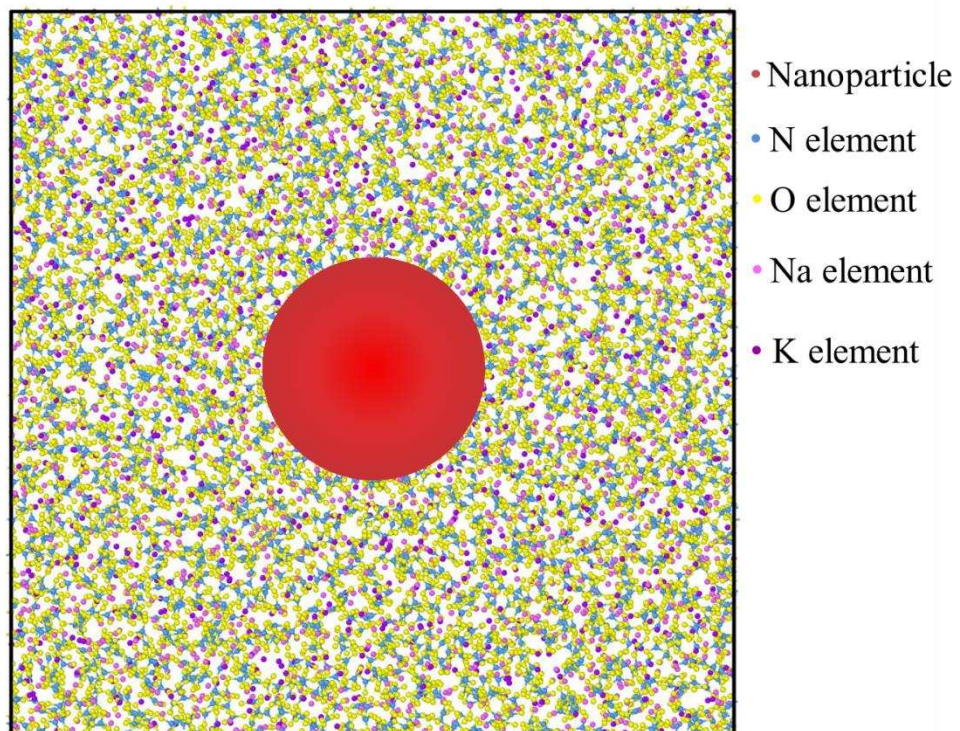
Fig. 1 Nanocomposite preparation procedure

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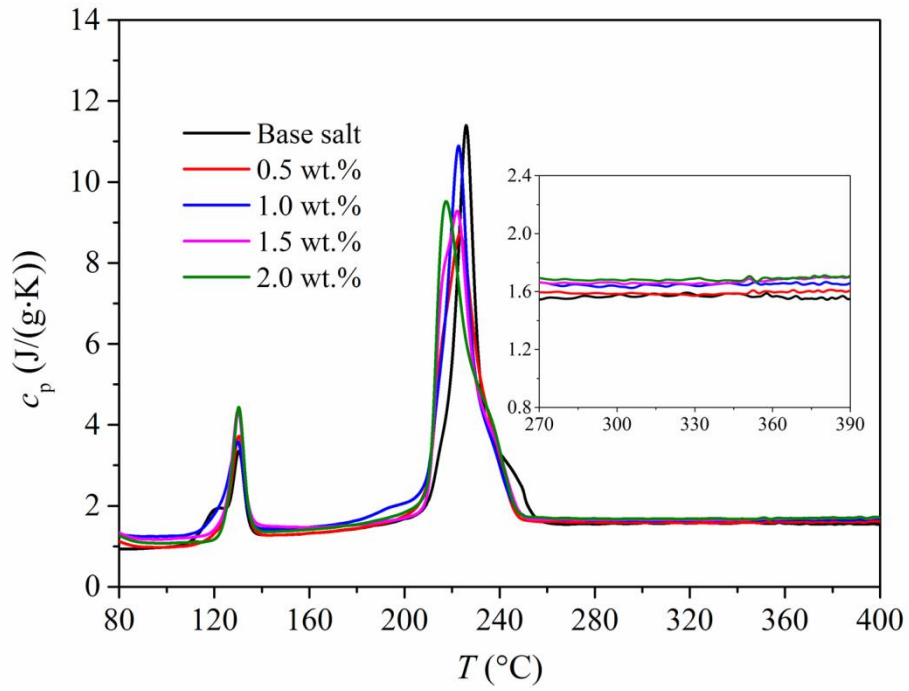
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Fig. 2 Simulation domain showing an Al_2O_3 nanoparticle surrounded by solar salt molecules

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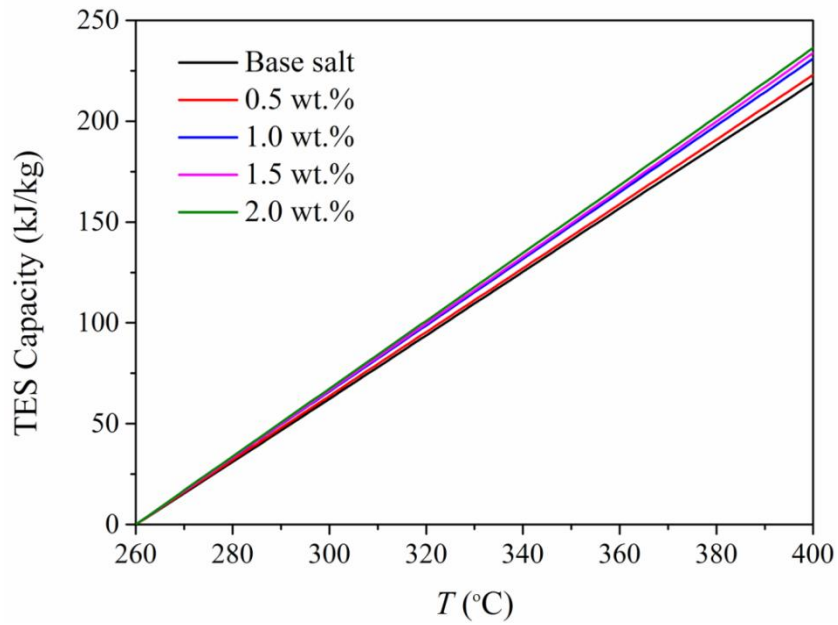
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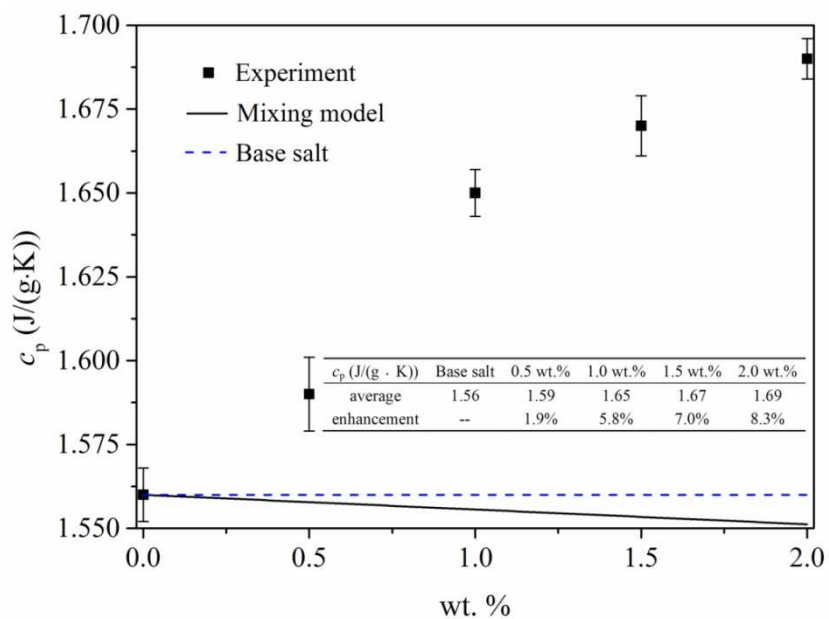
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Fig. 3 Variation in c_p with temperature for the pure base salt and at different nanoparticle mass concentrations (0.5%, 1.0%, 1.5%, and 2.0%)



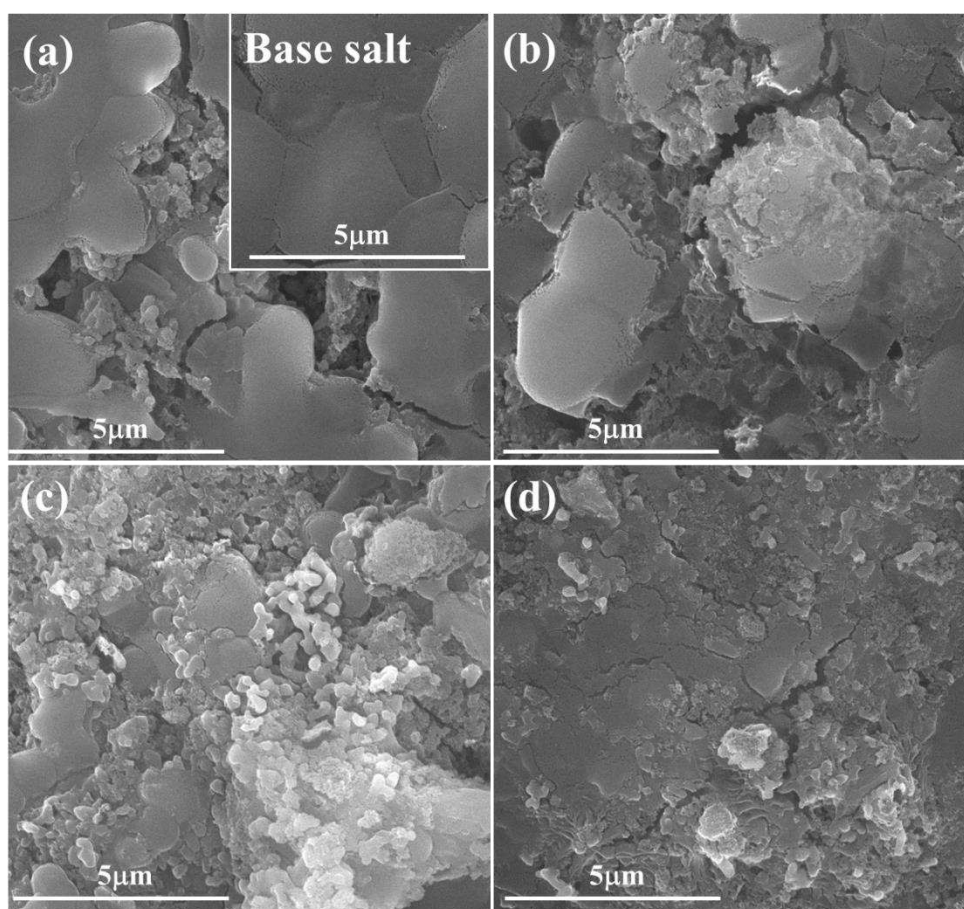
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Fig. 4 Variation of TES capacity with temperature, for pure base salt and after adding different amounts of nanoparticles.



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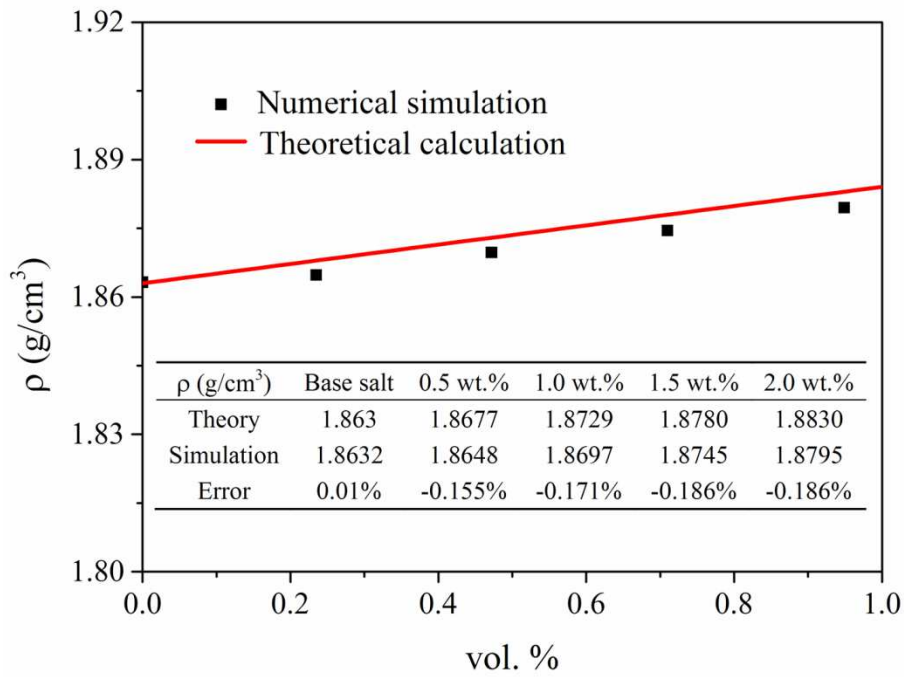
Fig. 5 Comparison of average experimental c_p values and the values predicted by the simple mixing model



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Fig. 6 SEM images of the salt with various nanoparticle concentrations after DSC measurement: (a) 0.5 wt.%, (b) 1.0 wt.%, (c) 1.5 wt.%, and (d) 2.0 wt.%.

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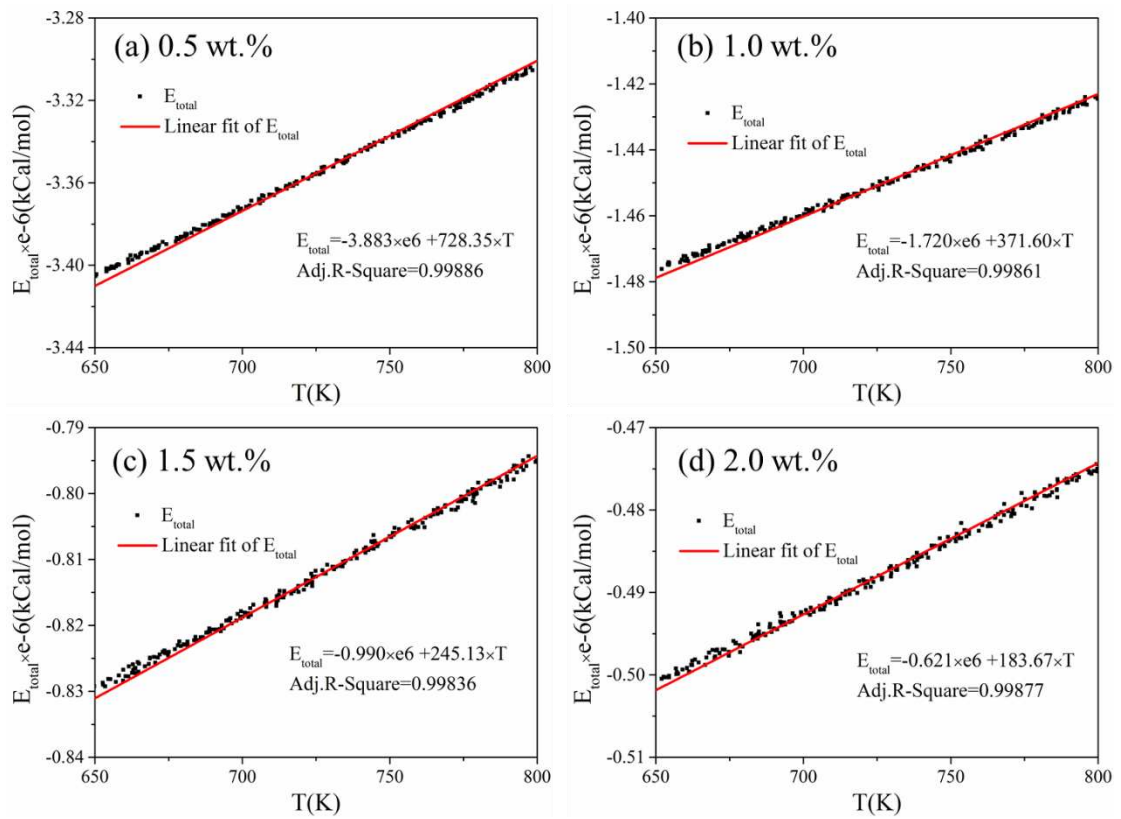
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515 Fig. 7 Comparison between simulations and theoretical calculations of the densities of a solar salt

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mixed with nanoparticles

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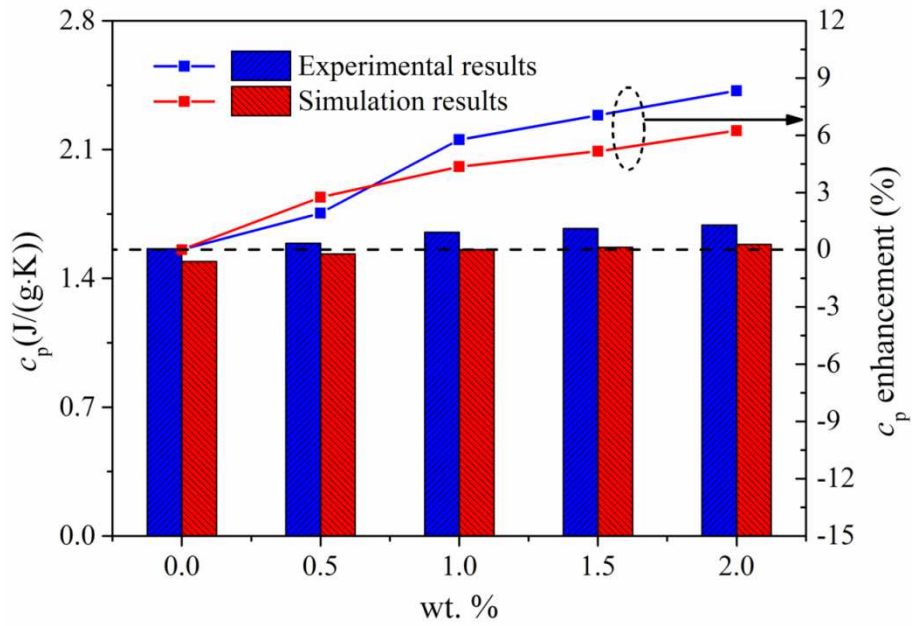
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519 Fig. 8 Total energy of the ensemble versus temperature: (a) 0.5 wt.%, (b) 1.0 wt.%, (c) 1.5 wt.%,

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and (d) 2.0 wt.%

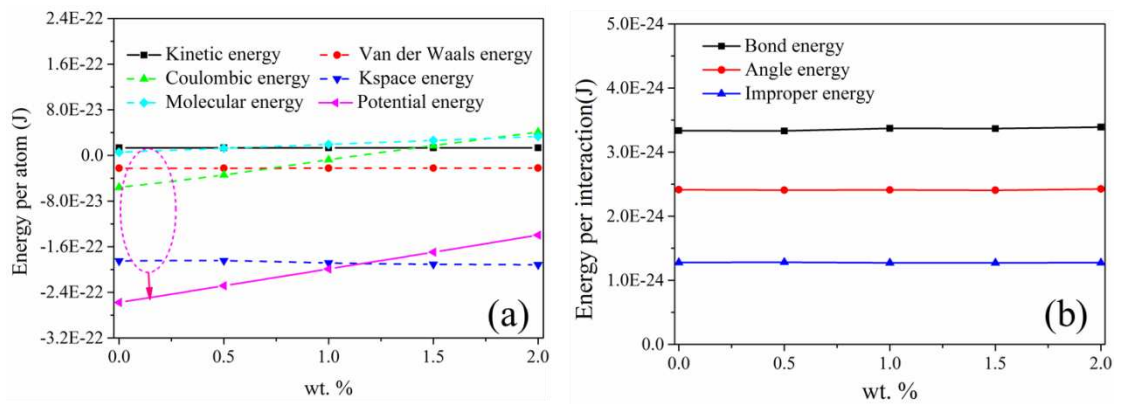
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524 Fig. 9 Experimental and simulated c_p values with different nanoparticle mass concentrations in the
525 salts

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528 Fig. 10 Potential and interaction energy analysis in the nanofluid system at 650 K

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Table 1 Simulation parameters for the MD simulation

Lennard-Jones constants							
Material	Interaction	ϵ [kcal/mol]	σ [Å]	Charge			
Al ₂ O ₃	Al-Al	0.040	4.053	+1.5			
	O-O	0.228	2.860	-1.0			
	N-N	0.167	3.501	+0.95			
Eutectic	O-O	0.228	2.860	-0.65			
	Na-Na	1.607	1.897	+1.0			
	K-K	5.451	3.197	+1.0			

Bonded interaction							
Material	Stretching		Bending		Improper torsional		
	k_s	r_0	k_b	θ_0	k_t	d_t	ϕ_t
Al ₂ O ₃	392.8	1.775	100.3	109.5	26.270	-1	2
Eutectic	525.0	1.268	105.0	120.0	26.270	-1	2

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Table 2 Experimental validation

Sample	Melting temperature (°C)			Enthalpy (J/g)		
	Experiment	Reference	Error	Experiment	Reference	Error
Sn	232.2	231.9	0.13%	59.28	60.5	-2.02%
Bi	271.7	271.4	0.11%	52.12	53.1	-1.85%

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Nomenclature

Symbol	Meaning
c_p	specific heat capacity, J/(g·K)
q	heat flow, W
m	weight, kg
E	potential energy, J
r	distance between two atoms, Å
q	charge of atom, C
k	constant
d	sign convention constant
T	temperature, K
V	volume, m ³
Q	thermal energy storage capacity, J/g
h	heat flow, mW/mg

Greek symbols

ε	potential well depth, kcal/mol
σ	finite distance for zero inter-particle potential, Å
θ	angle value, degrees
φ	volume fraction, -
ϕ	torsional angle, degrees
ρ	density, g/cm ³

Subscripts

s	sample
$sapp$	sapphire
b	bending
t	torsional

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