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Predicting Phase-Transition in Phase Change Materials Slurries: A Molecular Simulation Approach[1]

Predicción del cambio de fase en suspensiones de materiales de cambio de fase usando simulación molecular

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***Abstract*—Molecular dynamics simulations were performed to investigate the phase-transition behavior and thermophysical properties of octadecane–water phase-change slurries across the solid–liquid transition range of the paraffin phase. Octadecane was used as a model system to assess the capability of the method to describe phase transitions at the molecular level. Diffusion coefficients, radial distribution functions, specific volume, rotational time correlation functions, and thermal conductivity were systematically evaluated as functions of temperature. All descriptors consistently identified the transition between 308 and 318 K, confirming the coherence of the simulation framework. Although the simulated transition temperature was slightly higher than experimental values, the expected thermophysical trends were accurately reproduced, demonstrating that molecular dynamics is a reliable tool for analyzing and optimizing phase-change materials for thermal energy storage applications.**

***Keywords*—energy efficiency, molecular descriptors, molecular dynamics, phase-change materials.**

***Resumen*—Se realizaron simulaciones de dinámica molecular a diferentes temperaturas, para estudiar la transición de fase y las propiedades termo físicas de suspensiones de octadecano–agua como material modelo para la mejora de la eficiencia energética en materiales de construcción. Se analizaron coeficientes de difusión, funciones de distribución radial, volumen específico, correlaciones rotacionales y conductividad térmica en función de la temperatura. Todos estos descriptores identificaron de manera consistente la transición de fase entre 308 y 318 K, confirmando la validez del método utilizado. Aunque la temperatura de transición simulada es ligeramente superior a la experimental, se reprodujeron adecuadamente las propiedades termo físicas experimentales, lo cual demuestra que la dinámica molecular es una herramienta fiable para el análisis y optimización de materiales de almacenamiento térmico, cuya finalidad es la mejora de la eficiencia energética en el sector de la edificación.**

***Palabras Clave*—descriptores moleculares, dinámica molecular, eficiencia energética, materiales de cambio de fase.**

I. Introduction

PHASE-CHANGE materials (PCMs) have emerged as a cornerstone of modern energy-efficient technologies, particularly in the building and construction sectors. These materials offer a unique ability to absorb, store, and release energy through phase transitions, such as solid–liquid or solid–solid transformations, enabling effective thermal regulation across a wide range of applications [1]–[3]. During these transitions, PCMs can store substantial amounts of latent heat, making them highly effective in stabilizing indoor temperature fluctuations and reducing overall energy consumption. When integrated into construction elements such as walls, floors, and ceilings, PCMs enhance the thermal performance of buildings, thereby decreasing reliance on energy-intensive heating, ventilation, and air conditioning systems and contributing to the mitigation of greenhouse gas emissions [4]–[6].

PCMs are commonly classified as organic, inorganic, or eutectic materials, with organic paraffins being among the most widely used in sustainable building applications due to

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their favorable thermal properties, chemical stability, and compatibility with construction materials [7]–[9]. Paraffins, which are alkanes with the general formula C_nH_{2n+2}, offer the advantage of tunable melting temperatures through compositional control, making them particularly suitable for thermal energy management. Paraffins with melting points in the range of 290–303 K, such as octadecane ($C_{18}H_{38}$), are especially attractive for passive thermal energy storage in buildings, as their phase-transition temperatures closely match typical ambient conditions [10], [11].

Despite their advantages, paraffin-based PCMs suffer from inherent limitations, including low thermal conductivity and leakage during melting, which restrict their direct implementation in practical systems [12], [13]. To overcome these drawbacks, several strategies have been proposed, such as encapsulation, impregnation into porous matrices, and dispersion within polymeric supports [14]–[17]. Among these approaches, phase-change slurries (PCS), which consist of PCM capsules dispersed in a carrier fluid (commonly water), have gained significant attention. PCS combine latent and sensible heat storage, offering enhanced heat-transfer performance, improved flowability, and greater flexibility in thermal management applications [18]–[20]. The performance of PCS strongly depends on the design of the PCM capsules, typically involving core–shell structures that prevent leakage, enhance thermal conductivity, and ensure long-term stability [21]–[25].

While experimental studies have provided valuable insights into the macroscopic thermal and rheological behavior of PCS, molecular-level studies of phase transitions and transport properties remain insufficiently explored. Molecular dynamics (MD) simulations offer a powerful framework to address this limitation by enabling the identification of descriptors of structural, dynamic, and thermodynamic changes across phase transitions. However, despite their potential, MD simulations have so far been relatively underutilized in the systematic investigation of PCMs and PCS systems [26]–[28].

In this work, MD simulations are employed to investigate the thermal behavior and phase-transition characteristics of octadecane–water slurries. Thermophysical properties such as diffusion coefficients, radial distribution functions, specific volume, rotational time correlation functions, and thermal conductivity are analyzed over a temperature range encompassing the solid–liquid transition. Although octadecane–water slurries constitute a well-known and extensively studied system, they are deliberately selected here as a benchmark case to demonstrate how MD simulations can be systematically used to identify reliable molecular descriptors of phase transitions in PCM slurries. Rather than proposing a new material, the primary objective of this study is to establish and validate a transferable molecular simulation framework capable of capturing phase-transition behavior and thermophysical trends with predictive capability. By doing so, this work highlights the potential of MD simulations as a robust theoretical tool for the rational design and screening of novel PCMs and PCS, thereby supporting the development of more efficient and sustainable thermal energy storage solutions for building applications and beyond.

II. Materials and Methods

Three different models were constructed to investigate the thermal properties of the PCS. Their compositions are detailed in Table I, and their initial structures are shown in Fig. 1. All models were built using the Amorphous Cell module of the Materials Studio software [29]. A total of thirty-six molecules were employed to represent the amorphous structure of octadecane, which is adequate to reproduce its experimental properties, as confirmed by Rao et al. [30].

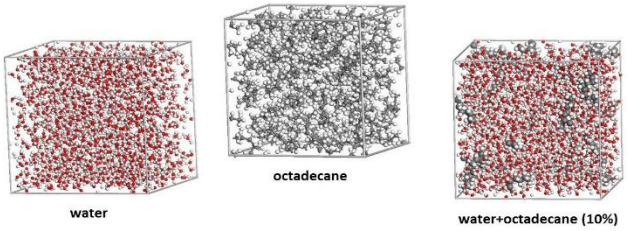


Fig. 1. Amorphous cell models of pure water, pure octadecane, and a 10% octadecane slurry used for the analysis of thermal transition properties.

Tabla I
Composition of the models used to characterize the PCS.

System	No. of water molecules	No. of octadecane molecules
Pure water	1490	0
Pure octadecane	0	36
Water+10% octadecane	1425	12

Density values of pure octadecane were calculated by simulation over a range of temperatures to validate the models employed in this study. Fig. 2 shows the resulting densities, together with literature data reported in [31] and [32] for comparison. The simulated results are in good agreement with previously published values, thereby confirming the reliability of the octadecane model used. The data points span the temperature range of approximately 270 K to 320 K, encompassing conditions under which phase transitions may occur.

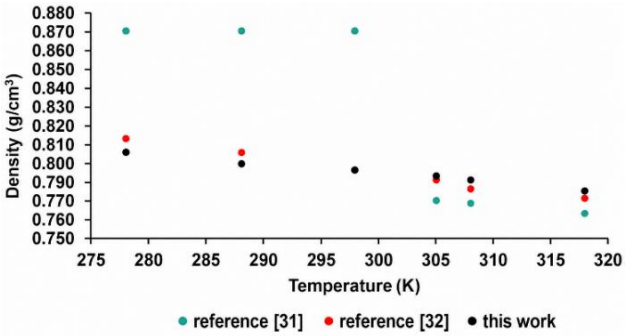


Fig. 2. Density of solid and liquid n-octadecane as a function of temperature, showing good agreement between the simulated values and previously reported experimental data.

MD simulations were performed using the Forcite module in Materials Studio [33] to investigate the thermal properties

of the models. Initial structures underwent energy minimization, followed by a 100 ps relaxation at 600 K. The systems were then equilibrated in the NVT ensemble for 1000 ps at target temperatures (see below). Thermo-physical properties were derived from subsequent 1000 ps NPT simulations, with data extracted from the final 200 ps. Temperature and pressure were controlled using a Nosé–Hoover thermostat [34] and a Berendsen barostat [35], respectively, with a time step of 1 fs.

Atomic interactions were described using the COMPASS II force field [36], which has been previously validated for alkane systems [26], [37]-[39]. To evaluate thermal transitions, MD simulations were carried out at temperatures below and above the melting point of octadecane. Phase transitions were assessed by analyzing changes in the properties written below.

A. Diffusion coefficient

The diffusion coefficient (D) of a system quantifies the mobility of its constituent particles and has been widely used to investigate phase transitions in various PCMs [26], [27], [38]-[40].

D can be determined from the slope of the mean squared displacement (MSD) versus time plot, assuming Fickian diffusion:

$$MSD = \sum_{i=1}^{N} < (ri(t) - ri(0))^2 >= 6.D.t \quad (1)$$

Where vector ri(0) represents the reference position of the i-th particle, while $r_i(t)$ de-notes the position of the same particle at time t.

B. Radial distribution function

The radial distribution function g(r) describes how particle density varies as a function of distance from a reference particle and, therefore, depends on temperature. As such, g(r) offers a statistical representation of the local packing and density within the system.

C. Specific volume

The specific volume represents the volume occupied by a unit mass of a substance and is defined as the reciprocal of its density. During a phase transition from solid to liquid, the specific volume undergoes a significant change, making it a useful indicator for identifying the point at which the phase change occurs.

D. Rotational time correlation function

The rotational diffusion of a molecule can be analyzed through its rotational time correlation function (RTCF), calculated for a vector that describes the molecular orientation. Accordingly, the first-rank RTCF (m_1) is expressed as:

$$m_1(t) = \langle u(t_0) \cdot u(t_0 + t) \rangle \quad (2)$$

Here, u(t) represents a unit vector that characterizes the molecular orientation at time t. In this study, u(t) is defined as the vector connecting the terminal carbon atoms of the octadecane molecule. For medium-length alkanes, this function decays exponentially as $\exp(-t/\tau_i)$ [41], where τ_i is the characteristic decay time.

E. Thermal conductivity

Thermal conductivity is a key property governing heat transfer in PCMs. Due to the limited experimental data on its variation during slurry phase transitions [42], MD simulations offer valuable insights. In this study, thermal conductivity was calculated using the Reverse Non-Equilibrium Molecular Dynamics (RNEMD) method developed by Müller-Plathe [43]. This approach induces a steady-state temperature gradient by exchanging velocities between the hottest and coldest particles in predefined slabs, generating a heat flux. Thermal conductivity is then obtained from the ratio of heat flux to the resulting temperature gradient, in accordance with Fourier's law.

These simulations enable a systematic evaluation of temperature-dependent structural, dynamic, and transport properties, discussed below.

III. Results and Discussion

In this section, the results obtained from the MD simulations are presented and discussed. The analysis focuses on the temperature-dependent behavior of octadecane and its slurry, with particular emphasis on identifying phase transitions.

A. Diffusion coefficient

The diffusion coefficients (D) for all structures examined in this study, calculated using Equation 1, are summarized in Table II. Fig. 3 shows the temperature dependence of D, highlighting how molecular diffusion evolves with temperature, a key factor in understanding the thermal behavior of the materials. The diffusion coefficient of octadecane remained nearly constant between 288 K and 308 K, followed by a marked increase from 308 K to 318 K, indicating a phase transition. This suggests the melting temperature of pure octadecane lies between 308 K and 318 K. The presence of water enhances octadecane diffusion, with both components exhibiting increased mobility at higher temperatures. These trends align with previous studies, where diffusion rises with temperature due to greater molecular motion [44].

B. Radial distribution function

To obtain information about the structure of pure octadecane, radial distribution functions (g(r)) were calculated at various temperatures. The results are shown in Fig. 4. The inset shows a magnified view of the first coordination peak, providing a detailed visualization to better analyze subtle temperature-dependent variations in its position and intensity. As the temperature increases, the intensity of the peaks decreases and shifts towards larger distances, indicating a rise in the disorder of the system.

TABLA II
DIFFUSION COEFFICIENTS FOR THE SYSTEMS INVESTIGATED IN THIS STUDY.

	D*10^5 (cm^2/s)					
Temperature (K)	278	288	298	305	308	318
pure water	5.091	5.163	5.980	6.569	7.165	8.176
pure octadecane	0.195	0.199	0.206	0.202	0.207	0.305
Water+10% octadecane	4.747[a] 0.794[b]	4.773[a] 0.820[b]	5.693[a] 0.896[b]	6.324[a] 0.954[b]	6.448[a] 1.022[b]	7.203[a] 1.290[b]

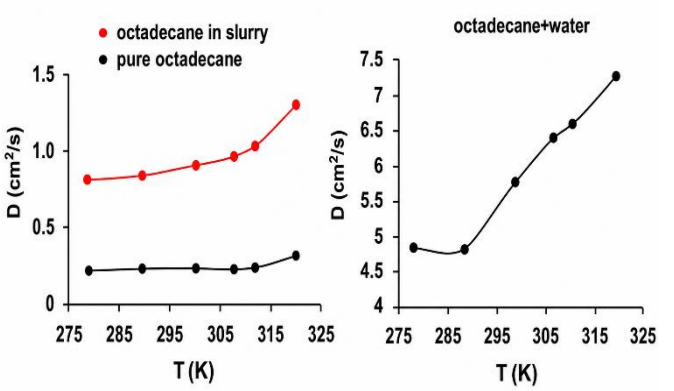


Fig. 3. Temperature dependence of the diffusion coefficient of octadecane (left) and slurry (right), revealing a sharp increase in molecular mobility across the solid–liquid phase-transition region.

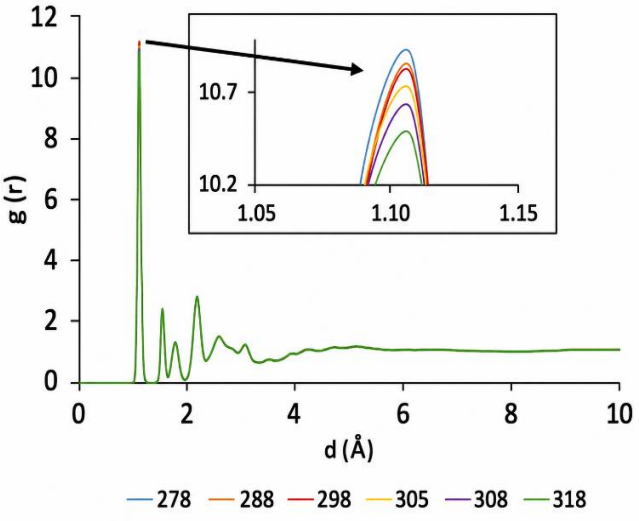


Fig. 4. Radial distribution functions of pure octadecane at various temperatures across the solid–liquid phase-transition region.

The progressive attenuation and shift of the structural peaks with increasing temperature confirm the loss of short-range order during melting, highlighting the ability of radial distribution functions to detect subtle structural signatures of the phase transition.

To further characterize the phase transition, the Wendt–Abraham parameter [44] was employed. This parameter is defined as:

$$R = \frac{g_{min}}{g_{max}} \tag{3}$$

Where *gmin* and *gmax* represent the intensities of the first minimum and first maximum of the radial distribution function, respectively.

R is plotted as a function of temperature in Fig. 5. There is a linear relationship between R and T, with the slope varying according to the state of octadecane. The intersection of the two curves indicates the temperature at which the phase change occurs. The obtained value, 308.33 K, aligns with the results from the analysis of the MSD plots. Experimental studies report melting temperatures for octadecane in the range of 298–302 K [12]. The slight overestimation observed in the simulations is a common feature of MD studies and can be attributed to finite system size effects, limited simulation timescales, and force-field approximations.

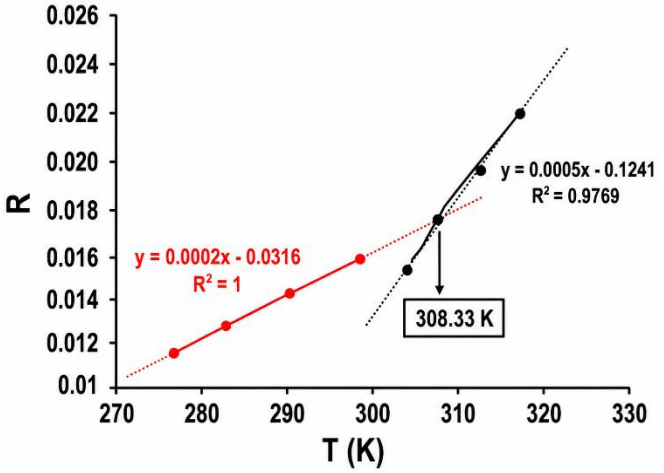


Fig. 5. Wendt–Abraham parameter as a function of temperature, highlighting a characteristic change that enables the identification of the solid–liquid phase-transition temperature.

C. *Specific volume*

The variation in the specific volume of pure octadecane with temperature is shown in Fig. 6.

As temperature increases from 278 to 318 K, the specific volume exhibits a monotonic upward trend, reflecting the expected thermal expansion behavior of the material. At lower temperatures, corresponding to the solid or semi-ordered phase, the specific volume increases gradually with temperature. As the system approaches and exceeds the melting region, a more pronounced increase is observed, indicating a transition toward a less ordered, liquid-like structure with increased molecular mobility and free volume.

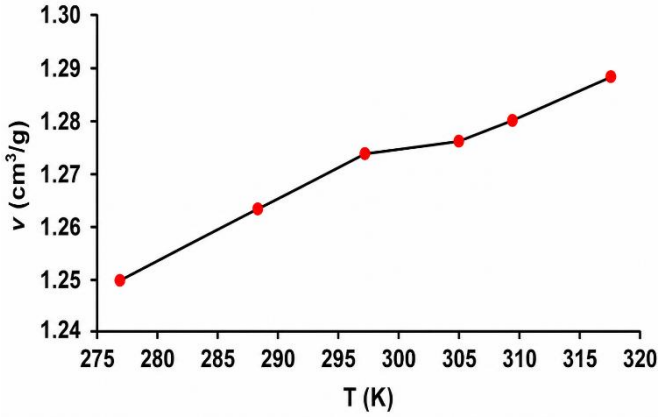
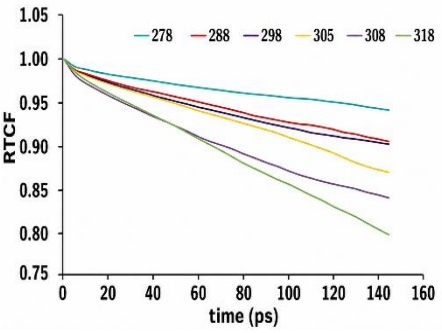


Fig. 6. Specific volume of octadecane as a function of temperature, exhibiting a change in slope associated with the solid–liquid phase transition.

This change in slope is consistent with the occurrence of a phase transition and highlights the sensitivity of specific volume as a thermodynamic descriptor for detecting melting behavior in phase-change materials such as octadecane. The obtained values are close to the experimental ones, which range from 1.28 to 1.35 cm³/g depending on temperature [12].

D. Rotational time correlation function

Fig. 7 presents the rotational time correlation functions (RTCFs) of pure octadecane on the left, along with the corresponding decay times on the right, evaluated at different temperatures. The RTCFs were qualitatively similar at different temperatures and were well fit by single exponentials, with decay times decreasing as the temperature increased. The RTCFs provide insight into the time-dependent molecular orientation and rotational dynamics of the system. The decay times represent the average duration required for the reorientation of the vector connecting the terminal carbon atoms of the octadecane molecule. As temperature increases, molecular motion becomes faster, leading to shorter decay times. At 318 K, octadecane was in a liquid state, allowing the molecules to rotate more freely and move more rapidly compared to lower temperatures. Zhang et al. [41] reported a decay time of 528 ps for eicosane (C20) at 323 K, which closely approximates the decay time calculated in this study for 318 K. The larger decay times observed at lower temperatures can be attributed to more restricted molecular motion in the solid state.



T (K)	τ_1 (ps)
278	2500
288	2000
298	1667
305	1111
308	1000
318	500

Fig. 7. RTCF of octadecane molecules at different temperatures, showing accelerated rotational dynamics upon transition to the liquid state. (left) and decay times (right) of pure octadecane at different temperatures.

The temperature-dependent decrease in rotational relaxation times reflects the increasing freedom of molecular reorientation upon melting, offering complementary insight into the dynamic aspects of the phase transition beyond translational motion.

E. Thermal conductivity

The thermal conductivities (k) of water, octadecane, and the slurry as functions of temperature are shown in Fig. 8.

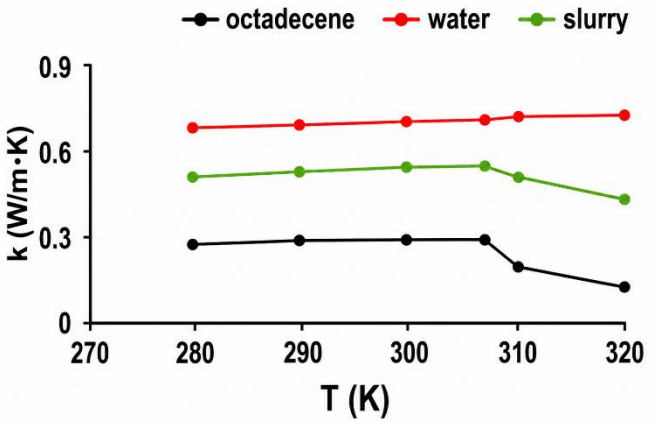


Fig. 8. Temperature dependence of the thermal conductivity of water, octadecane, and octadecane–water slurries, showing a non-monotonic behavior for the PCM-containing systems across the phase-transition regions

Fig. 8 shows that as temperature increases, the thermal conductivity of pure water rises slightly. The simulated thermal conductivity of water is in good agreement with experimental values, which are reported to be around 0.56–0.63 W m^{-1} K^{-1} in the temperature range considered, and correctly reproduces the slight increase with temperature. In contrast, for the octadecane-containing models, thermal conductivity increases with temperature up to the phase-transition point and then decreases beyond it. The obtained thermal conductivity values are close to experimental data, which report values between 0.2 and 0.35 W m^{-1} K^{-1} depending on phase and temperature, with higher values in the solid state and lower values in the liquid state [12]. The thermal conductivity of the slurry is lower than that of pure water due to the significantly lower thermal conductivity of octadecane compared to water. Above the melting point of octadecane, the thermal conductivity of the slurry also decreases, like pure octadecane. These trends are also confirmed by experimental studies on microencapsulated paraffin slurries [45]–[47].

IV. Conclusions

In this study, MD simulations were applied to systematically analyze the phase-transition behavior and thermophysical properties of octadecane–water slurries. Although octadecane represents a well-established PCM, it was deliberately employed as a reference system to demonstrate the ability of MD simulations to capture phase-transition phenomena and to identify reliable molecular-level descriptors relevant to slurry-based thermal material.

The solid–liquid transition of octadecane was consistently detected within the temperature range of 308–318 K using a combination of independent indicators, including diffusion coefficients, radial distribution functions, specific volume,

rotational time correlation functions, and thermal conductivity. The agreement among structural, dynamic, and transport properties confirms that MD simulations provide a coherent and internally consistent description of phase transitions in PCMs. The simulations further reveal the role of water in enhancing molecular mobility and modulating heat-transport behavior, highlighting the potential of atomistic modeling to analyze PCM–fluid interactions in slurry systems.

Although the predicted transition temperature slightly overestimates experimental values, this discrepancy is within the expected limits of MD simulations and does not compromise the accuracy of the reproduced thermophysical trends.

Beyond the specific system studied, this work establishes a transferable simulation framework that can be readily extended to more complex PCM formulations and represents a critical tool for the next step: modeling core-shell encapsulated slurries to elucidate confinement effects and interfacial heat transfer mechanisms at the molecular level, ultimately guiding material design By enabling the identification of key molecular descriptors governing phase transitions and thermal transport, MD simulations offer a rational basis for the screening and optimization of PCMs, supporting the development of advanced thermal energy storage systems for energy-efficient applications. In conclusion, this approach may significantly reduce experimental trial-and-error in the development of advanced PCM-based systems.

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REFERENCIAS

[1] Barbi, S., Barbieri, F., Marinelli, S., Rimini, B., Merchiori, S., Bottarelli, M., and Montorsi, M., (2022). Phase change material evolution in thermal energy storage systems for the building sector, with a focus on ground-coupled heat pumps. Polymers, 14, 620. 10.3390/polym14030620.

[2] Rostami, S., Afrand, M., Shahsavar, A., Sheikholeslami, M., Kalbasi, R., Aghakhani, S., Safdari, M., and Oztop, H.F., (2020). A review of melting and freezing processes of PCM/nano-PCM and their application in energy storage. Energy, 211, 118698. 10.1016/j.energy.2020.118698.

[3] Silva, T., Vicente, R., Amaral, C., and Figueiredo, A., (2016). Thermal performance of a window shutter containing PCM: numerical validation and experimental analysis. Appl. Energy, 179, 64. 10.1016/j.apenergy.2016.06.126.

[4] Kant, K., Shukla, A., and Sharma, A., (2017). Heat transfer studies of building brick containing phase change materials. Sol. Energy, 155, 1233. 10.1016/j.solener.2017.07.072.

[5] Faraj, K., Khaled, M., Faraj, J., Hachem, F., and Castelain, C., (2021). A review on phase change materials for thermal energy storage in buildings: heating and hybrid applications. Energy Storage, 33, 101913. 10.1016/j.est.2020.101913.

[6] Gholamibozanjani, G., and Farid, M., (2020). A comparison between passive and active PCM systems applied to buildings. J. Renew. Sustain. Energy, 162, 112. 10.1016/j.renene.2020.08.007.

[7] Lamrani, B., Johannes, K., and Kuznik, F., (2021). Phase change materials integrated into building walls: an updated review. Renew. Sustain. Energy Rev., 140, 110751. 10.1016/j.rser.2021.110751.

[8] Razak, R.A., Khang, A.C., Al Bakri, M.M., Yahya, Z., Junaidi, S., Muhamad, K., and Mohd, N.A., (2019). Paraffin as a phase change material in concrete for enhancing thermal energy storage. IOP Conf. Ser.: Mater. Sci. Eng., Lodz, Poland. 10.1088/1757-899X/551/1/012093.

[9] Bharathiraja, R., Ramkumar, T., Selvakumar, M., Radhika, N., Praveenkumar, N., Mohanraj, M., and Mohamed Iqbal Shajahan, (2025). Advancements in paraffin wax phase change materials: a comprehensive review of enhancement techniques and thermal storage applications. Thermochim. Acta, 753, 180129. 10.1016/j.tca.2024.180129.

[10] Hassan, F., Jamil, F., Hussain, A., Ali, H.M., Jangua, M.M., Khushnood, S., Farhan, M., Altaf, K., Said, Z., and Li, C., (2022). Recent advancements in latent heat phase change materials and their applications for thermal energy storage and buildings: a state-of-the-art review. Sustain. Energy Technol. Assess., 49, 101646. 10.1016/j.seta.2021.101646.

[11] Kenisarin, M., Mahkamov, K., Kahvash, F., and Makhkamova, I., (2019). Enhancing thermal conductivity of paraffin wax 53–57 °C using expanded graphite. Sol. Energy Mater. Sol. Cells, 200, 110026. 10.1016/j.solmat.2019.110026.

[12] Faden, M., Höhlein, S., Wanner, J., König-Haagen, A., and Brüggemann, D., (2019). Review of thermophysical property data of n-octadecane for phase-change studies. Materials, 12, 2974. 10.3390/ma12182974. DOI: 10.3390/ma12182974.

[13] Berardi, U., and Gallardo, A.A., (2019). Properties of concretes enhanced with phase change materials for building applications. Energy Build., 199, 402. 10.1016/j.enbuild.2019.07.014.

[14] Hassan, A., Laghari, M.S., and Rashid, Y., (2016). Micro-encapsulated phase change materials: a review of encapsulation, safety and thermal characteristics. Sustainability, 8, 1046. 10.3390/su8101046.

[15] Rathore, P.K.S., and Shukla, S.K., (2020). An experimental evaluation of thermal behavior of the building envelope using macroencapsulated PCM for energy savings. Renew. Energy, 149, 1300. 10.1016/j.renene.2019.10.121.

[16] Chen, Y., Li, X., Gao, J., Yang, M., Liu, Y., and Tang, X., (2021). Carbon layer-modified mesoporous silica supporter for PEG to improve the thermal properties of composite phase change material. J. Mater. Sci., 56, 5786. 10.1007/s10853-020-05658-0.

[17] Chen, K., Yu, X., Tian, C., and Wang, J., (2014). Preparation and characterization of form-stable paraffin/polyurethane composites as phase change materials for thermal energy storage. Energy Convers. Manag., 77, 13. 10.1016/j.enconman.2013.09.006.

[18] Borri, E., Hua, N., Sciacovelli, A., Wu, D., Ding, Y., Li, Y., Brancato, V., Zhang, Y., Frazzica, A., Li, W., Yu, Z., Milian, Y.E., Ushak, S., Grágeda, M., and Cabeza, L.F., (2022). Phase change slurries for cooling and storage: an overview of research trends and gaps. Energies, 15, 6873. 10.3390/en15196873.

[19] McPhee, H., Soni, V., Saber, S., Zargartalebi, M., Riordon, J., Holmes, M., Toews, M., and Sinton, D., (2023). Rheological behavior of phase change slurries for thermal energy applications. Langmuir, 39, 119. 10.1021/acs.langmuir.2c02279.

[20] Zhang, P., Qiu, Z., and He, M., (2014). Review on microencapsulated phase change materials (MPCM) slurries: materials, rheological behavior and applications. Adv. Mater. Res., 953, 1109. 10.4028/www.scientific.net/AMR.953-954.1109.

[21] Zhang, H., Sun, S., Wang, X., and Wu, D., (2011). Fabrication of microencapsulated phase change materials based on n-octadecane core and silica shell through interfacial polycondensation. Colloids Surf. A, 389, 104. 10.1016/j.colsurfa.2011.08.042.

[22] Khan, Z., Khan, Z., and Ghafoor, A., (2016). A review of performance enhancement of PCM based latent heat storage system within the context of materials, thermal stability and compatibility. Energy Convers. Manag., 115, 132. 10.1016/j.enconman.2016.02.045.

[23] Cao, L., Tang, F., and Fang, G., (2014). Synthesis and characterization of microencapsulated paraffin with titanium dioxide shell as shape-stabilized thermal energy storage materials in buildings. Energy Build., 72, 31. 10.1016/j.enbuild.2013.12.018.

[24] Li, B., Liu, T., Hu, L., Wang, Y., and Gao, L., (2013). Fabrication and properties of microencapsulated paraffin@SiO2 phase change composite for thermal energy storage. ACS Sustain. Chem. Eng., 1, 374. 10.1021/sc300082m.

[25] Yesilyurt, M.K., and Comakli, O., (2023). Encapsulated phase change material slurries as working fluid in novel photovoltaic thermal liquid systems: a comprehensive review. Iran J. Sci. Technol. Trans. Mech. Eng., 47, 1275. 10.1007/s40997-023-00599-0.

[26] Rao, Z., Wang, S., Wu, M., Zhang, Y., and Li, F., (2012). Molecular dynamics simulations of melting behavior of alkane as phase change materials slurry. Energy Convers. Manag., 64, 152. 10.1016/j.enconman.2012.04.015.

[27] Wang, Y., Chen, Z., and Ling, X., (2016). A molecular dynamics study of nano-encapsulated phase change material slurry. Appl. Therm. Eng., 98, 835. 10.1016/j.applthermaleng.2015.11.085.

[28] Tafrishi, H., Sadeghzadeh, S., and Ahmadi, R., (2022). Molecular dynamics simulations of phase change materials for thermal energy storage: a review. RSC Adv., 12, 14776. 10.1039/D2RA02021H.

[29] BIOVIA, (2025). Materials Studio Amorphous Cell. [Online]. Available: [https://www.3ds.com/fileadmin/PRODUCTS-SERVICES/BIOVIA/PDF/biovia-material] (https://www.3ds.com/fileadmin/PRODUCTS-SERVICES/BIOVIA/PDF/biovia-material) studio-amorphous-cell.pdf.

[30] Rao, Z.H., Wang, S.F., and Zhang, Y.L., (2012). Simulation of heat dissipation with phase change material for cylindrical power battery. J. Energy Inst., 85, 38. 10.1179/1743967112Z.0000000007.

[31] Vélez, C., Khayet, M., and Ortiz de Zárate, J.M., (2015). Temperature-dependent thermal properties of solid/liquid phase change even-numbered n-alkanes: n-hexadecane, n-octadecane and n-eicosane. Appl. Energy, 143, 383. 10.1016/j.apenergy.2015.01.037.

[32] Rao, Z., Wang, S., and Peng, F., (2012). Self-diffusion of the nano-encapsulated phase change materials: a molecular dynamics study. Appl. Energy, 100, 303. 10.1016/j.apenergy.2012.05.029.

[33] BIOVIA, (2025). Materials Studio Forcite. [Online]. Available: https://www.3ds.com/fileadmin/PRODUCTS-SERVICES/BIOVIA/PDF/biovia-material-studio-forcite.pdf

[34] Hoover, W.G., (1985). Canonical dynamics: equilibrium phase-space distributions. Phys. Rev. A, 31, 1695. 10.1103/PhysRevA.31.1695.

[35] Berendsen, H.J.C., Postma, J.P.M., Van Gunsteren, W.F., DiNola, A., and Haak, J.R., (1984). Molecular dynamics with coupling to an external bath. Chem. Phys., 81, 3684. 10.1063/1.448118.

[36] Sun, H., Ren, P., and Fried, J.R., (1998). The COMPASS force field: parameterization and validation for phosphazenes. Comput. Theor. Polym. Sci., 8, 229. 10.1016/S1089-3156(98)00042-7.

[37] Yang, J.S., Yang, C.L., Wang, M.S., Chen, B.D., and Ma, X.G., (2011). Crystallization of alkane melts induced by carbon nanotubes and graphene nanosheets: a molecular dynamics simulation study. Phys. Chem. Chem. Phys., 13, 15476. 10.1039/C1CP21067F.

[38] Liu, X., Lin, C., and Rao, Z., (2017). Diffusion and thermal conductivity of the mixture of paraffin and polystyrene for thermal energy storage: a molecular dynamics study. J. Energy Inst., 90, 534. 10.1016/j.joei.2016.05.006.

[39] Nie, C., Tong, X., and Peng, D., (2015). Paraffin confined in carbon nanotubes as nanoencapsulated phase change materials: experimental and molecular dynamics studies. RSC Adv., 5, 92812. 10.1039/C5RA18898E.

[40] Abbaspour, M., Jorabchi, M.N., Akbarzadeh, H., and Ebrahimnejad, A., (2021). Investigation of the thermal properties of phase change materials encapsulated in capped carbon nanotubes using molecular dynamics simulations. RSC Adv., 11, 24594. 10.1039/D1RA04052E.

[41] Zhang, Y., Venable, R.M., and Pastor, R.W., (1996). Molecular dynamics simulations of neat alkanes: the viscosity dependence of rotational relaxation. J. Phys. Chem., 100, 2652. 10.1021/jp952134n.

[42] Dutkowski, K., and Kruzel, M., (2021). Experimental investigation of the apparent thermal conductivity of microencapsulated phase-change-material slurry at the phase-transition temperature. Materials, 14, 4124. 10.3390/ma14154124.

[43] Müller-Plathe, F. (1997). A simple nonequilibrium molecular dynamics method for calculating the thermal conductivity. J. Chem. Phys., 106, 6082. 10.1063/1.473271.

[44] Zhang, G.H., and Zhao, C.Y., (2011). Thermal and rheological properties of microencapsulated phase change materials. Renew. Energy, 36, 2959. 10.1016/j.renene.2011.03.045.

[45] Karaipekli, A., Erdogan, T., and Barlak, S., (2019). The stability and thermophysical properties of a thermal fluid containing surface functionalized nanoencapsulated PCM. Thermochim. Acta, 682, 178406. 10.1016/j.tca.2019.178406.

[46] Joseph, M., and Sajith, V., (2019). An investigation on heat transfer performance of polystyrene encapsulated n-octadecane based nanofluid in square channel. Appl. Therm. Eng., 147, 756. 10.1016/j.applthermaleng.2018.10.126.

[47] Al-Waeli, A.H.A., Sopian, K., Chaichan, M.T., Kazem, H.A., Ibrahim, A., Mat, S., and Ruslan, M.H., (2017). Evaluation of the nanofluid and nano-PCM based photovoltaic thermal (PVT) system: an experimental study. Energy Convers. Manag., 151, 69

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