Understanding phase transition between the liquid and gaseous states has gained significant interest, and has been ubiquitously observed in many places ranging from natural systems to water–energy nexus and thermal management applications. Phase transition phenomena at liquid–vapor interfaces are greatly governed by intermolecular-level kinetics, which requires the use of empirical parameters in continuum-level relations to explain the discrete nature of molecular particles. Despite its significance, it has been a great challenge to find detailed expressions of empirical parameters such as accommodation coefficients, which represent the probabilities for phase transition of liquid or vapor molecules at the interface. Here, direct statistical measurements of accommodation coefficients are reported by tracking the trajectories of liquid and vapor molecules in molecular simulations. The measurements reveal that evaporation and condensation coefficients are different by $\approx 50\%$, whereas they have been assumed to be equal in most previous studies. Then, the indirect measurement method is studied from a perspective of theoretical genetics based on the diffusion approximation. A good agreement between two approaches suggests that diffusion approximation can contribute to provide empirical parameters with a cost-effective method.

1. Introduction

Phase transition describes changes between solid, liquid, and gaseous states of matter with given thermodynamic conditions, representing the evolution of thermodynamic state of molecules. Phase transition phenomena can be ubiquitously observed in many natural processes ranging from agricultural systems and hydrogeology to water cycles as well as thermal management devices. In nature, transpiration is an evaporation process by which moisture is carried through plants from roots to microscale pores on the underside of leaves where it changes to vapor and is released to the atmosphere. Evaporated vapor molecules are captured on insect or plant surfaces that possess microscale structures through condensation process. In modern engineering, there have been numerous efforts to develop thermal management devices that facilitate evaporation or condensation phase transition processes by installing nanostructures. Despite the significance of the phase transition process in many applications that have implemented nanostructures, it has been challenging to completely understand nanoscale phase transition process at the molecular level.

Phase transition process between individual particles has been traditionally explained by continuum theories. A classical Schrage model derived from kinetic theory explains the evaporation mass and energy fluxes at a liquid–vapor interface, which requires the precise measurement of interfacial thermofluidic parameters such as temperature and pressure. In addition, the Schrage model and many other theories require the use of empirical parameters to be implemented in the models to account for intermolecular properties at the vapor–liquid interface. For example, evaporation and condensation accommodation coefficients represent the probabilities for a liquid particle to evaporate and for a vapor particle to condense at the interface. The coefficients are often assumed to be a constant or equal with a wide range spanning three orders of magnitude ($10^{-3}$ to $1$) in many cases, although the coefficients possess distinctive values for evaporation and condensation and vary for different boundary conditions in reality. Therefore, the continuum theories with those assumptions often fail to conserve momentum or energy equations, requiring explicit expressions for accommodation coefficients. Unfortunately, it has been extremely challenging to obtain such expressions theoretically or experimentally from previous studies.

With the aim of identifying accommodation coefficients during phase transition, theoretical genetics might play a key role.
The similarity of interactions between two phases and gene types. a) Illustration displays the exchange between liquid and vapor molecules near the liquid–vapor interface and corresponding accommodation coefficients \( \alpha \). The subscripts “e” and “c” represent evaporation and condensation, respectively. b) Illustration shows mutation processes in a gene population. Coefficients \( \alpha_{AB} \) and \( \alpha_{BA} \) denote the mutation rates from A to B and B to A, respectively.

in understanding phase transition phenomena while the interactions between liquid and vapor molecules (Figure 1a) could be analogous to the interactions in a population with two types of genes in theoretical genetics (Figure 1b). The change in the molecule numbers in each phase is similar to the change in the number of gene types during evolution. For example, as the liquid evaporates, the number of liquid molecules decreases in the same manner as one type of gene undergoes gradual loss during genetics evolution. This implies that accommodation coefficients in phase transition can be comparable with transition rates between two types of genes. Despite these similarities between interface interactions of two phases and gene populations of two gene types, there have been no such efforts to relate the phase transition process to well-developed genetic theories. The similarities motivate us to utilize simplified models along with molecular-level calculations to advance the understanding about the intertwined phase transition physics at the interface from a new perspective. This approach might offer an alternative, indirect method that predicts the accommodation coefficients for given thermodynamics conditions without the necessity to track the trajectories of each individual particle, which eventuates in lowering computational costs.

Computational techniques based on molecular dynamics (MD) simulation models are presented in this paper to investigate thin-film phase transition phenomena, along with the computations of accommodation coefficients that are responsible for the intrinsic intermolecular dynamics. The results reveal the significant differences between evaporation and condensation accommodation coefficients as well as a strong temperature dependency. The results from direct calculations of molecular models are consistent with a much simpler and cost-effective, indirect measurements from a perspective of genetics theory based on the diffusion approximation (DA). The analysis is further verified by comparing the evaporation rates from molecular models to those from continuum-level theory. New discoveries about the similarity between genes’ evolution and molecule–molecule interaction will allow us to predict the accommodation coefficients for given thermodynamics conditions at relatively lower costs.

2. Simulation Methods

In this study, MD simulation models are performed by using large-scale atomic/molecular massively parallel simulator (LAMMPS). LAMMPS uses Verlet integrator algorithm to solve the equations of motion. A time step of 1 fs is chosen for the computations to ensure stability of the motion of molecules. TIP4P potential is employed to represent water molecules, which provides a reasonably accurate view of thermodynamic properties of water and its experimental structural shape. The TIP4P model consists of four different sites: two sites for positive charged hydrogen atoms, one negative charged site, and another Lennard–Jones (LJ) site for oxygen atom. SHAKE algorithm used keeps harmonic O–H and H–H bonds, and H–O–H angle to be rigid to prevent vibrational motions. Particle-particle-particle-mesh (PPPM) solver calculates long range coulombic interactions. Interactions between water and metal molecules are defined by LJ potential and by assuming interactions only between O and Cu atoms. The Cu–Cu interactions are modeled by using embedded atom model (EAM).

The simulation unit cell is a 7.23 nm \( \times \) 3.61 nm \( \times \) 22.92 nm rectangular box, as illustrated in Figure 2c. The unit cell consists of 6400 Cu molecules arranged in a face centered cubic (FCC) structure with a lattice constant of 3.615 Å at the top and the bottom of the simulation cell. The outermost two layers of copper are fixed to ensure that the simulation unit cell has a constant volume during the simulations. A thin layer of water of 2, 3, and 5 nm consisting of 1740, 2610, and 4350 water molecules, respectively, is placed on the copper surface. Periodic boundary conditions are applied in all directions to ensure particle interactions across the boundary of the unit cell. Prior to all simulations, the entire system is equilibrated for 1 ns in a constant-temperature, constant-volume ensemble (NVT) where the atom number, the
Figure 2. Solid–liquid–vapor interfacial kinetics in evaporation process. a) The schematic shows the example of nanostructures in contact with liquid water. The installation of nanostructures helps liquid wick through the nanostructures with minimum meniscus thickness, enabling thin film evaporation.\textsuperscript{[32]} b) Detailed illustration of a thin liquid film at the molecular scale: “incident” represents the molecules moving toward the interface from one phase to the another phase; “reflection” describes the incident molecules reflecting back to their original phase; and “accommodation” represents the incident molecules that are accommodated by the opposite phase. Interfacial region is identified by an imaginary plane called the $\Gamma$-plane, which is located at a range of distances ($\sigma$ to $3\sigma$) from the moving interface $\delta(t)$, where the interface has a density of 0.4 g cm$^{-3}$. c) Computational unit cell with dimensions $a \times b \times c$ is illustrated. Thin liquid film with an initial thickness of $\delta_i$ is placed on a copper surface. Unit cell shows hot and cold surfaces with temperatures $T_h$ and $T_c$ that act as a heater and condenser, respectively.

volume, and the temperature of the system are constant at 300 K, in each case. Then, the phase transition process of the water film is studied in a constant-energy, constant-volume ensemble (NVE) under various elevated temperatures of the copper surface ranging from 400 to 500 K for different cases. The elevated temperature is defined by increasing the temperature of the copper surface through Brendson scheme, whereas the temperature of the top copper surface is maintained at 300 K as the collector of the evaporated water molecules. The high temperatures are selected to expedite the slow evaporation process and to save computational cost. It should be noted that evaporation only occurs at the liquid–vapor interface due to strong attraction forces between molecules and extremely small thicknesses of liquid film, while boiling is not observed. In addition, we should note that we consider the closed cell with low temperature and high temperature reservoirs at the both ends in order to minimize the effects of the cell dimensions on the calculated accommodation coefficients.

To calculate thermophysical properties, we discretize the unit cell into small 3D grids of 2 Å × 2 Å × 2 Å and calculate average properties in each grid. Figure S1a, Supporting Information, shows the discretized domain in the $x$-$z$ plane. The averaged values of each property, such as density, temperature, kinetic, and potential energies, are obtained and averaged for all the particles that are located inside one of the grids. To define the interface between water and vapor regimes, the density distribution profile is used (Figure S1c, Supporting Information). The density changes from $\approx 0.8$ g cm$^{-3}$ (liquid density) to $\approx 0$ g cm$^{-3}$, whereas the average of the two densities (0.4 g cm$^{-3}$) is used as the criterion to define the water–vapor interface.

3. Results and Discussions

3.1. Direct Statistical Measurements of Accommodation Coefficients from MD Models

MD simulation models calculate the trajectories of atoms and molecules over time and hence provide the detailed physics of phase transition at interfacial regions between two phases.\textsuperscript{[44–50]} To gain insights into the atomistic picture of phase transition process, we use MD models that simulate an evaporating thin liquid film on nanostructures, as illustrated in Figure 2a. The detailed view in Figure 2b shows the interactions between liquid and vapor molecules at the interface, representing accommodation and reflection processes. We build a unit cell shown in Figure 2c containing liquid molecules on a solid surface for different temperatures $T_i$.

MD simulations when combined with the tools of statistical mechanics of particles\textsuperscript{[51]} can provide individuals’ thermodynamic and kinetic properties in the two-phase system\textsuperscript{[53–56]} enabling us to directly measure the accommodation coefficients. To do this, the trajectories of all molecules are tracked with respect to an imaginary plane,\textsuperscript{[16,17]} called the $\Gamma$-plane during the MD computations shown in Figure 2c (see Supporting Information 2 for more information on molecule trajectories). The
The histogram shows that most of the incident liquid molecules are recorded for all incident liquid molecules in the system, denoted as the “reflection time interval” or $\Delta t$. The probability histogram of the reflection time interval is thereby plotted, as shown in Figure 3a for $T_{liq} = 500$ K and $\delta_i = 3$ nm. The histogram shows that most of the incident liquid molecules immediately return to their original phase (liquid in this case) in short time intervals (the peak of the bar plot is associated with small time intervals in Figure 3a), whereas a limited number of incident molecules maintain the new phase (vapor) for longer time intervals. By integrating the probability histogram, the total reflection probability is obtained for varying time intervals, as shown in the secondary axis in Figure 3a. Subtracting the total reflection probability from 1 provides the accommodation probability for various reflection time intervals, as shown in Figure 3b. As the accommodation probability stabilizes with time, the corresponding value in the plateaued region (the changes are smaller than 0.5%) can be considered as the evaporation accommodation coefficient $\alpha_e = 1 - \lim_{\Delta t \to \infty} \frac{N_{ref,V}}{N_{inc,V}}$. Figure 3c shows the evaporation accommodation coefficients $\alpha_e$ for varying temperature $T_{liq}$ and liquid thickness $\delta_i$. The same approach is used to calculate condensation accommodation coefficient $\alpha_c$ by tracking the trajectories of all incident vapor molecules (Figure 3d inset). Consequently, the condensation accommodation coefficients $\alpha_c = 1 - \lim_{\Delta t \to \infty} \frac{N_{ref,L}}{N_{inc,L}}$ for various temperatures and liquid thicknesses are obtained and shown in Figure 3e,f. The plots indicate that the values of evaporation and condensation accommodation coefficients are different by 41% to 55%. This distinction between the values is often overlooked and the coefficients are assumed to be equal in most previous studies[22–30] despite the significance of the accurate estimates of those values in the Schrage model. The higher values of evaporation accommodation coefficients indicate that the incident liquid molecules are more probable to vaporize and stay in the acquired vapor phase as they evaporate. Due to the continuous condensation of vapor molecules on the cold surface at the top, the vapor density and the collision rates between molecules are low. Hence, the probability \( \Gamma \)-plane is placed at distances in the range of $\sigma$ to $3\sigma$—LJ characteristic distance ($\sigma = 3.16$ Å for O–O interactions)$^{[21]}$—above the liquid–vapor interface $\delta(t)$. It is worth noting that the location of $\Gamma$-plane continuously changes as the interfacial plane recedes during evaporation processes. First, the trajectories of all incident liquid molecules (Figure 3a inset) that are moving toward and crossing the $\Gamma$-plane from liquid phase and the number $N_{inc,L}$ is obtained. The interval times for an incident liquid molecule to cross the $\Gamma$-plane and reflect back to its original $\Gamma$-plane is placed at distances in the range of $\sigma$ to $3\sigma$—LJ characteristic distance ($\sigma = 3.16$ Å for O–O interactions)$^{[21]}$—above the liquid–vapor interface $\delta(t)$.
of reflection for evaporating liquid molecules is much smaller than the condensing vapor molecules. It should be noted that the values of accommodation coefficients are calculated for the interface at highly non-equilibrium conditions.

The accommodation coefficients are reported for varying temperature $T_0$, ranging from 400 to 500 K and liquid thickness $\delta = 2, 3$, and 5 nm. Both accommodation coefficients linearly decrease as the temperature increases, as shown in Figure 3c,f. The results are consistent with the previous values reported in elsewhere.\[19,48,57\] The temperature dependency can be explained by the mobility of the interfacial molecules. As the mobility increases with higher temperatures, a large number of collisions between the molecules occur, which directly increase the number of reflected molecules after collisions. The mobility at higher temperatures also lowers the normal translational energy of incident molecules, showing a decreasing trend in the normal component of the velocity. The molecules with low normal velocities often stay near the liquid–vapor interface and easily reflect back to the original state. Since accommodation coefficients are inversely proportional to the number of reflected molecules, these accommodation coefficients will decrease with increasing temperatures. In addition, the accommodation coefficients confirm the independence on the liquid film thickness by showing <6% deviations in Figure 3c,f.

3.2. Interpretation of Accommodation Coefficients from the Perspective of Theoretical Genetics

Although the direct statistical measurements of MD models present the accurate estimates of accommodation coefficients, the expensive computational costs make it difficult to be widely used in many applications. Instead, the similarities between a genetic evolution and a phase transition process might allow us to analogize accommodation coefficients based on the DA, which can significantly reduce the complexity of calculations in a system with multiple parameters.\[52\] In theoretical genetics, one representative theoretical model, the Wright–Fisher, provides mathematical explanations for genetic mechanisms\[58–61\] by tracking the frequencies of different alleles in a population: If the population consists of $N$ individuals, either type $A$ or $B$, the state $X_A$ describes the presence of $X_A$ individuals of type $A$, and state $X_B$ describes the presence of individuals of type $B$ where $N = X_A + X_B$. During the genetic evolution, the ratio of the number of type $A$ individuals $X_A$ to the total population size $N$ is expressed as $p = \frac{X_A}{N}$ and possesses discrete values between 0 and 1 (e.g., 0/N, 1/N, ..., N/N). For the case of a large population with small mutation rates between types $A$ and $B$,\[61\] $p$ can be assumed as a continuous variable between 0 and 1, called the continuous approximation. This allows us to explain the evolution process by using the DA model that describes a continuous stochastic process.\[63–65\] For this, the Kolmogorov’s forward partial differential equation is considered\[61\]

$$\frac{\partial f (p, t)}{\partial t} = - \frac{\partial}{\partial p} \left[ \mu (p) f (p, t) \right] + \frac{1}{2} \frac{\partial^2}{\partial p^2} \left[ \sigma^2 (p) f (p, t) \right]$$

(1)

where $f(p, t)$ is the probability density function (that records the rate at which a certain value of $p$ is possessed), $\mu(p)$ is the diffusion drift, and $\sigma^2 (p)$ is the diffusion variance. Due to the continuous approximation, diffusion drift and variance can be expressed as

$$\mu (p) = -\alpha_{AB} p + \alpha_{BA} (1 - p)$$

(2)

$$\sigma^2 (p) = p (1 - p)$$

(3)

where the $\alpha_{AB}$ or $\alpha_{BA}$ are the mutation rates to describe the changes from type $A$ to type $B$ or type $B$ to type $A$ at an instant of time, respectively. Representation of the mutations between type $A$ and type $B$ is illustrated in Figure 1b. Therefore, the steady state diffusion equation is

$$\frac{\partial}{\partial p} \left[ (1 - p) f (p, t) \right] = \frac{1}{2} \frac{\partial^2}{\partial p^2} \left[ (1 - p) f (p, t) \right]$$

(4)

where $f(p, t)$ is rewritten as $f(p)$ to represent the steady solution for the diffusion, and the general solution of Equation (4) follows

$$f (p) = C p^{2\alpha_{AB} - 1} (1 - p)^{2\alpha_{BA} - 1}$$

(5)

where $C$ is the scaling factor.

In phase transition physics, we similarly consider the evaporating liquid film as a system containing two types of molecules, type $L$ (i.e., liquid) and type $V$ (i.e., vapor) where the change in the number of type $L$ (or type $V$) molecules with time can provide accurate estimations on evaporation (or condensation) rates, as illustrated in Figure 1a. At each instant of time, the ratio of the number of type $L$ molecules $X_L$ to the total number of molecules $N$ is referred as $p = \frac{X_L}{N}$ and has discrete values between 0 and 1. Mutation rates from type $L$ to type $V$ and type $V$ to type $L$ can be used to describe evaporation and condensation accommodation coefficients, respectively. Based on the continuous approximation explained in theoretical genetics, the DA can be thereby valid to explain the evaporation and condensation process. For such a system with large number of particles and small accommodation coefficients, the general solution of diffusion equation in the form of Equation (5) can be rewritten as

$$f (p) = C p^{2\alpha_L - 1} (1 - p)^{2\alpha_V - 1}$$

(6)

where $\alpha_L$ and $\alpha_V$ are evaporation and condensation accommodation, respectively.

The changes in $X_L$ during evaporation can be obtained from MD simulation models for varying time, and $p$ is thereby calculated for varying simulation times. A representative profile of $p$ is shown in Figure 4a inset for the case of $T_0 = 440$ K. As can be seen, the initial value of 1 of $p$ starts decreasing at a small rate as evaporation process starts in the beginning of the simulation. Later, the probability density of $p$ decreases with an almost linear trend and eventually plateaus toward a zero value. As $p$ changes with time, the evaporation process can be categorized into three different regions: the onset, the steady, and the dry-out regions. Probability densities and variations of $p$ with time for other temperatures in the range of 400 to 500 K are shown in Supporting Information 4. The resulting probability density in Figure 4a shows a U shape with highest values near the ends. Therefore, the lower and upper bounds (where the population
Figure 4. Indirect measurements of accommodation coefficients from a perspective of genetics theory. a) Bar plot shows the probability density of \( p \) with time. Inset shows the fraction of type \( L \) molecules to the total number of molecules \( p = X_l / N \) at the bottom surface over time at \( T_h = 440 \) K for a thin film with \( \delta_i = 3 \) nm. Three regions of the onset, the steady, and the dry-out are identified during the evaporation process as the time increases. By comparing the probability density of \( p \) obtained from MD and DA models, fitting parameters and accommodation coefficients are calculated. The resulting b) evaporation and c) condensation accommodation coefficients calculated from MD and DA models agree well by showing 20–39% deviations.

Figure 5. Evaporative rates obtained by tracking molecule trajectories and by implementing accommodation coefficients to the Schrage model. a) Evolution of evaporation rates for varying surface temperatures \( T_h \) where the liquid film thickness is 3 nm. The evaporation rates rapidly increase initially in the onset region, plateau in the steady state region, and decrease down to zero as all the water molecules are absorbed to the cold surface in the dry-out region. b) Average evaporation rates \( \dot{m}_{\text{MD}}' \) during the steady-state region are mainly governed by temperature rather than water film thickness. c) Evaporation rates of \( \dot{m}_{\text{Schrage-MD}}' \) and \( \dot{m}_{\text{Schrage-DA}}' \) from the Schrage equation are presented where the accommodation coefficients from MD trajectories and DA models are used, respectively. The colormap shows the range of evaporation rates if the accommodation coefficients between 0.1 and 1 are used in the Schrage model.

3.3. Direct Estimation of Evaporation Rates: Using MD Models

MD models provide the detailed information of the number of molecules in each phase at different times, enabling the direct calculation of evaporation rate from MD models \( \dot{m}_{\text{MD}}'' \). The evaporation rates can be calculated based on the rate at which the number of liquid molecules decreases at each instant of time

\[
\dot{m}_{\text{MD}}'' = \frac{\Delta N_l}{\Delta t} \frac{M_l}{N_{AV}} \frac{1}{A_{LV}}.
\]

where \( N_l \) is the number of liquid molecules at each time step; \( \Delta t \) is the time interval for which evaporation is calculated; and \( N_{AV} \), \( M_l \), and \( A_{LV} \) are the Avogadro’s number, water molar weight, and liquid–vapor interface area, respectively. The time-dependent evaporation rates for the \( \delta_i = 3 \) nm film are plotted in Figure 5a for \( T_h \) ranging from 400 to 500 K. The evaporation rates for all temperatures initially increase, then get stabilized in a steady state region, and finally decrease down to zero. At the beginning of the process in the onset region, fast evaporation is observed due to the lower vapor density and thereby low rates of collisions. As the evaporation continues, the thin film thickness \( \delta(t) \) decreases, eventualing in a higher disjoining pressure between liquid and solid molecules that suppresses evaporation. The suppressing effect of disjoining pressure balances with the net
evaporation rates in the steady region. As the thin film thickness further decreases, disjoining pressure gets stronger to complete the evaporation. The evaporation rates finally decrease toward zero, indicating the dry-out of the solid surface. The evaporation rates \( m'' \) are calculated by averaging the rates within the steady state region within 20% of the maximum value and are reported in Figure 5b, which shows the independence to the liquid film thickness.

For the validation purpose, we further calculate the evaporation rates \( m'' \) using the Schrage equation by implementing the accommodation coefficients calculated through the MD and DA models in earlier section

\[
\begin{align*}
    m''_{\text{Schrage}} &= \frac{2}{2 - \alpha_e} \sqrt{\frac{M}{2\pi R}} \left( a_e \frac{P_{eq}}{\sqrt{T_L}} - a_v \frac{P_v}{\sqrt{T_v}} \right) \\
    m''_{\text{MD}} &= \frac{2}{2 - \alpha_e} \sqrt{\frac{M}{2\pi R}} \left( a_e \frac{P_{eq}}{\sqrt{T_L}} - a_v \frac{P_v}{\sqrt{T_v}} \right) \\
    m''_{\text{DA}} &= \frac{2}{2 - \alpha_e} \sqrt{\frac{M}{2\pi R}} \left( a_e \frac{P_{eq}}{\sqrt{T_L}} - a_v \frac{P_v}{\sqrt{T_v}} \right)
\end{align*}
\]

where \( P_{eq} \) and \( P_v \) represent the equilibrium pressure and vapor pressure, respectively. The equilibrium pressure \( P_{eq} \) is calculated by using separate MD models (see Supporting Information for the detailed calculations of thermophysical properties). The combination of thermophysical properties and accommodation coefficients \( \alpha_{MD} \) and \( \alpha_{DA} \) in Figure 3c,f computes the evaporation rates \( m''_{\text{MD}} \) and \( m''_{\text{DA}} \) based on the Schrage equation, as shown in Figure 5c. Similarly, the combination of thermophysical properties and accommodation coefficients \( \alpha_{MD} \) and \( \alpha_{DA} \) calculates the evaporation rates \( m''_{\text{MD}} \) and \( m''_{\text{DA}} \). The comparison between MD trajectories and DA models shows a good agreement with 20% and 39% deviations for evaporation and condensation, respectively, whereas the range of accommodation coefficients between 0.1 and 1 shows large deviations, which have been commonly used in previous studies. Since the obtained results are independent of the initial liquid thickness, only the values related to \( \delta = 3 \text{ nm} \) are presented in Figure 5.

4. Conclusion

In this work, the direct statistical measurements of accommodation coefficients by tracking the trajectories of liquid and vapor molecules in molecular simulations are reported. Further, a classical population genetics model is suggested for the first time as an indirect measurement method to explain molecular-level transitions from liquid to vapor phases. The cost-effective, indirect measurements based on the genetics theory successfully predict accommodation coefficients to be used in continuum-level models. The computational results reveal the significance of temperatures in determining the overall evaporation performances. The resulting evaporation and condensation coefficients are different by \( \approx 50\% \), while they have been assumed to be equal in most previous studies. The development of new approach can contribute to provide empirical parameters required for the analysis of phase transition phenomenon.

Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest

The authors declare no conflict of interest.

Keywords

accommodation coefficients, evaporation, molecular dynamics, phase transition, theoretical genetics

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