

Energy Conversion Characteristics of Coalescence-Induced Jumping of Translating and Rolling Nanodroplets on Superhydrophobic Surfaces

Xiaodong Wang, Shaofei Zheng, Yifeng Wang, and Fangfang Xie

Abstract—Coalescence-induced droplet jumping is a key mechanism for passive phase-change transport and energy-efficient liquid removal on superhydrophobic surfaces. While static droplet coalescence has been widely studied, the energy conversion behavior of moving droplets, especially under rolling motion, remains unclear at the nanoscale. In this work, molecular dynamics simulations are conducted to investigate the coalescence-induced jumping of translating and rolling nanodroplets over a range of Weber numbers. Results show that translational motion mainly compresses the coalescence timescale, while the dimensionless jumping velocity remains nearly constant due to the interfacial energy constraint on vertical kinetic energy. In contrast, rolling motion enhances vertical momentum establishment and modifies directional energy partitioning. Although the absolute vertical kinetic energy increases under rolling conditions, its conversion efficiency decreases with increasing initial velocity, while horizontal and total energy conversion efficiencies exhibit a rise-then-decline trend, indicating an optimal inertial regime. These findings elucidate how motion mode governs energy redistribution during droplet coalescence and provide nanoscale insight for improving energy-efficient phase-change transport.

Index Terms—Coalescence-induced jumping, energy conversion efficiency, nanodroplet dynamics, translating and rolling motion, molecular dynamics simulations.

ABBREVIATION

MD	molecular dynamics
FCC	face-centered cubic
mW	monatomic water
We	Weber number
Oh	Ohnesorge number

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1. INTRODUCTION

When two or more droplets coalesce on a superhydrophobic surface, a portion of the excess surface energy released during coalescence can be converted into the kinetic energy of the merged droplet. This phenomenon, commonly referred to as *coalescence-induced droplet jumping* [1], [2], [3], [4], arises from the rapid reduction of interfacial area and the associated capillary-driven recoil. Owing to its ability to enable spontaneous droplet removal without external actuation, coalescence-induced jumping has attracted extensive attention in recent years and has been widely explored in applications such as self-cleaning surfaces [5], [6], self-sustained condensers [7], enhancement of dropwise condensation heat transfer [8], [9], and anti-icing technologies [10], [11].

Extensive investigations have been conducted on coalescence-induced jumping of static droplets on planar substrates, addressing multiple aspects such as energy conversion efficiency, surface wettability, jumping velocity, droplet size, and initial droplet configuration. Boreyko and Chen [4] experimentally introduced a dimensionless jumping velocity defined as $v^* = v_{\text{ex}}/v_i$, where v_{ex} is the measured departure velocity and $v_i = (\gamma/\rho r)^{1/2}$ is the inertial-capillary velocity scale, with γ denoting the liquid-vapor surface tension, ρ the liquid density, and r the average droplet radius. This scaling framework has since served as a fundamental reference for subsequent studies. Using three-dimensional numerical simulations, Nam et al. [12] analyzed the dynamics of droplet coalescence and jumping on superhydrophobic surfaces and reported that approximately half of the released surface energy is converted into kinetic energy during coalescence. Liu et al. [13] further proposed a physical model for self-propelled jumping and demonstrated numerically that, for two identical static droplets coalescing on an ideal non-wetting surface (contact angle of 180°), the released surface energy is partitioned into translational kinetic energy and oscillatory energy. Based on the energy conversion efficiency relationship $E_k/\Delta E_s \approx v_j^{*2}$ (with $v_j^{*2} \approx 0.2$), where ΔE_s represents the excess surface energy, and E_k denote the kinetic energy at the departure moment. They showed that only a small fraction of the excess surface

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energy is converted into upward translational motion, while the majority is stored in oscillatory modes and eventually dissipated.

To characterize the competition between inertial-capillary and viscous-capillary regimes, Liu et al. [14] introduced the Ohnesorge number (Oh) = $\mu/(\rho\gamma r)^{1/2}$, where μ is the dynamic viscosity. Subsequently, Xie et al. [15] incorporated the droplet radius ratio r^* and proposed modified inertial-capillary velocity and effective Ohnesorge number scalings, establishing a generalized framework for understanding coalescence between unequal-sized droplets. Molecular dynamics (MD) studies further revealed that size asymmetry also plays a crucial role at the nanoscale: When the radius ratio reaches 2, droplet rebound no longer occurs. For two identical static droplets, the jumping velocity follows the classical inertial-capillary scaling $v_j \propto U = (\gamma/\rho r)^{1/2}$ [16]. In contrast, for droplets of unequal size, the departure velocity is strongly influenced by the smaller droplet due to adhesion effects, and decreases monotonically with increasing size ratio until jumping is completely suppressed [17], [18].

The lateral momentum transfer associated with coalescing droplets, arising from the sustained horizontal motion of the merged droplet, plays a critical role in enhancing the performance of practical applications. However, most previous studies have focused primarily on static droplets, whereas investigations involving moving droplets remain comparatively limited. Li et al. [19] reported that the initial velocity of a moving droplet promotes liquid bridge expansion and enhances droplet deformation, leading to asymmetric morphologies during coalescence. Moreover, the presence of initial motion increases the overall energy conversion efficiency, defined as $\varepsilon_{\text{total}} = (E_{k,x} + E_{k,y})/(\Delta E_s + E_{k,\text{ini}})$, where $E_{k,\text{ini}}$ is the initial kinetic energy of the moving droplet, and $E_{k,x}$ and $E_{k,y}$ denote the horizontal and vertical kinetic energies at the departure moment, respectively. They observed that the vertical kinetic energy initially exhibits weak dependence on the initial velocity; however, when the velocity exceeds 0.35 m/s, $E_{k,y}$ increases, displaying a trend of slight reduction followed by rapid growth. Enright et al. [20] combined experiments and numerical simulations to demonstrate that coalescence-induced droplet jumping is intrinsically limited in efficiency. Only approximately 6% of the excess surface energy can be converted into translational kinetic energy. For example, at $Oh = 0.12$, the energy conversion efficiency was reported to be as low as 1.8%. As the Ohnesorge number increases, the efficiency decreases further due to enhanced viscous dissipation. This work provided important insights into the intrinsic limitations of coalescence-induced jumping and established an upper bound for the attainable departure velocity on flat hydrophobic surfaces. Although the kinetic energy characteristics of coalescence-induced jumping of translating droplets have been revealed, such studies still fail to match the non-translational motion modes of droplets in realistic application scenarios, and the core issue of low energy conversion efficiency has not yet been reasonably explained.

Compared with purely translational droplets, rolling droplets with an imposed horizontal velocity are more representative of realistic operating conditions. In practical scenarios such as condensation and droplet transport, droplets frequently acquire rotational motion while translating across the surface. Liu et al. [21] investigated frontal coalescence between a rolling droplet and a stationary droplet and demonstrated that the droplet radius ratio significantly influences the dependence of vertical jumping velocity on the dimensionless initial velocity. When the radius ratio (r_s/r_m) exceeds 0.8, the vertical departure velocity first increases and then decreases with increasing initial velocity, with a critical velocity given by $v_c^* = 0.9(r_s/r_m)$. In contrast, for radius ratios smaller than 0.8, increasing the initial velocity consistently promotes the vertical component. They further showed that the horizontal departure velocity scales approximately linearly with the dimensionless initial velocity. As the initial velocity increases, the jumping angle decreases, and the departure direction becomes progressively more parallel to the substrate; this effect is more pronounced for larger radius ratios. Yilbas et al. [22] conducted a comparative study on the droplet rolling dynamics over grooved hydrophobic surfaces, clarified the influences and regulatory effects of grooved substrates on the unidirectional rolling characteristics, rotational speed and droplet cluster evolution of droplets, and revealed that interfacial adhesion force acts as the core factor governing the droplet rolling dynamic behaviors on grooved hydrophobic surfaces. Subsequently, Liu et al. [23] employed single-camera defocused imaging to accurately reconstruct the three-dimensional jumping trajectories of merged droplets. Their results revealed that, under non-frontal coalescence conditions, the initial velocity and the lateral offset jointly determine the rotational intensity of the merged droplet. A higher initial velocity was found to suppress the vertical velocity component, particularly when the lateral offset was large, whereas its influence on the horizontal velocity was comparatively weak. At the nanoscale, Liang et al. [24] employed molecular dynamics simulations to show that coalescence-induced jumping shares qualitative similarities with micron-scale droplets. During coalescence, the released surface energy is partially converted into the translational kinetic energy of the merged droplet. However, for droplets with a radius of 18 nm, the center-of-mass kinetic energy at departure accounts for only about 1.3% of the excess surface energy, while nearly 99% is dissipated through internal viscous effects. Due to the larger effective Ohnesorge number at the nanoscale, viscous dissipation becomes more significant, resulting in substantially lower energy conversion efficiency. Nevertheless, research on nanoscale rolling droplets still remains a critical gap.

In summary, substantial differences exist between translational and rolling droplets when they interact with a stationary droplet. For translational droplets, low-velocity impact may preserve a nearly spherical morphology, whereas at high Weber numbers (We) splashing and pronounced lateral spreading can occur, leading to the so-called “pancake bounce

ing” behavior [25]. In contrast, rolling droplets tend to spread more readily along the substrate, thereby increasing the contact area. This effect becomes more pronounced at higher initial velocities, which facilitates droplet coalescence by enhancing interfacial contact. From an energy perspective, the dissipation mechanisms governing the two modes also differ. For translational droplets, energy loss in the early stage is primarily associated with viscous dissipation, which reduces the sum of surface and kinetic energies; as the velocity increases, inertial effects become more significant and dominate the energy redistribution process [26], [27]. The dynamics of rolling droplets are inherently more complex. In addition to viscous dissipation, rotational motion introduces angular kinetic energy, interfacial friction with the substrate, and wettability-dependent interactions, all of which influence the partitioning and dissipation of energy during coalescence.

Although considerable progress has been made in understanding coalescence-induced jumping between moving and stationary droplets, a systematic understanding of rolling-droplet-involved coalescence remains lacking, particularly at the nanoscale, where the distinct regulatory effects of translational and rolling motion modes on coalescence dynamics and directional energy conversion have not been clearly distinguished. Key issues such as liquid bridge formation, the evolution of morphological anisotropy, and the partitioning of kinetic energy between lateral and vertical channels have not yet been fully clarified and warrant further investigation. To address these gaps, the present study employs molecular dynamics simulations to construct a coalescence system consisting of equal-sized nanodroplets on a superhydrophobic Pt substrate. Two distinct motion modes, pure translation and rolling, are considered, and their coalescence-induced jumping behaviors are systematically examined over a range of initial velocities corresponding to different Weber numbers. By comparing the dynamic evolution, geometric characteristics, and energy distribution under these two modes, this work aims to elucidate the nanoscale physical mechanisms governing coalescence-induced jumping of moving droplets, with particular emphasis on rolling droplets, to fill the research gap of nanoscale rolling droplet coalescence dynamics and provide targeted fundamental insight for the optimization of energy-efficient passive droplet removal strategies in practical phase-change transport scenarios.

II. SIMULATION METHOD AND MODEL

A. Computational Domain and Initial Configuration

Molecular dynamics simulations were performed using the LAMMPS package to investigate coalescence-induced jumping of nanoscale water droplets on a platinum (Pt) substrate. The initial configuration consists of a horizontally positioned Pt substrate and two spherical water droplets of equal radius (5 nm). The droplets are initially separated along the horizontal direction with a center-to-center gap of 114 Å; the left

droplet is assigned motion while the right droplet remains stationary. The complete initial setup is illustrated in Fig. 1. The Pt substrate has a thickness of 1.1838 nm and contains 99,660 Pt atoms. To preserve crystallographic consistency, Pt atoms are arranged in a face-centered cubic (FCC) lattice with a lattice constant of 3.946 Å. The initial droplet structures are generated using an FCC arrangement of water particles with a lattice constant of 4.927 Å to construct spherical droplets.

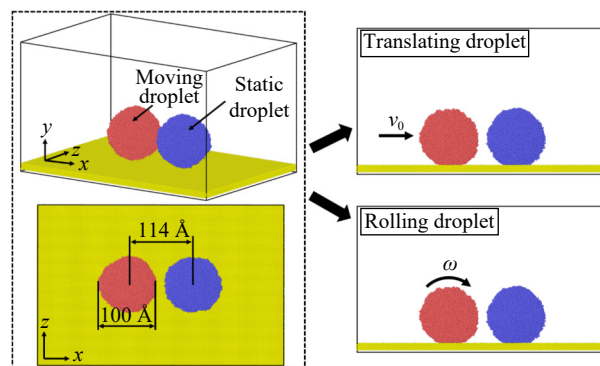


Fig. 1. Schematic illustration of the molecular dynamics simulation setup for coalescence-induced jumping between a moving droplet and a stationary droplet on a Pt substrate.

To minimize finite-size effects and approximate an effectively extended interface, periodic boundary conditions are imposed in the x , y , and z directions. The bottommost layer of Pt atoms is fixed in the y direction to provide structural rigidity, while the remaining Pt atoms are maintained at 300 K using a thermostat to represent thermal coupling with the surrounding environment.

B. Molecular Model and Interatomic Interactions

To balance computational efficiency with the accurate representation of interfacial dynamics, water molecules are modeled using the coarse-grained monatomic water (mW) potential [28], in which each water molecule is represented as a single interaction site. Despite its simplified description, the mW model has been shown to reproduce essential macroscopic properties of water, including surface tension, density, and viscosity, while significantly reducing computational cost. Owing to these advantages, it has been widely adopted in simulations of droplet dynamics and phase-transition phenomena at the nanoscale.

Interatomic interactions are described using the Lennard–Jones (L–J) potential [29], expressed as:

$$V_{ij} = 4\varepsilon[(\sigma/R)^{12} - (\sigma/R)^6] \quad (1)$$

where R denotes the interparticle distance, while ε and σ represent the potential well depth and characteristic length scale, respectively. The Lennard–Jones parameters used in this study are as follows: for Pt–Pt interactions, $\varepsilon_{\text{Pt–Pt}} = 0.69375$ eV and $\sigma_{\text{Pt–Pt}} = 2.47$ Å; and for Pt–water interactions, $\varepsilon_{\text{Pt–water}} = 0.002$ eV and $\sigma_{\text{Pt–water}} = 2.8155$ Å. A relatively weak Pt–water

interaction strength is deliberately adopted to realize a low-adhesion boundary condition, thereby mimicking a superhydrophobic substrate and facilitating droplet detachment during coalescence-induced jumping [30].

C. Simulation Procedure and Operating Conditions

The simulations are conducted in two successive stages: system equilibration and coalescence-induced jumping dynamics.

(1) Equilibration stage

The system is first relaxed in the canonical (NVT) ensemble at 300 K to ensure thermal stability. To prevent artificial droplet detachment caused by abrupt initial interactions, the Pt–water interaction strength is gradually adjusted during equilibration. Specifically, a relatively stronger interaction is applied during the first 0.2 ns to enhance initial adhesion and stabilize the droplets on the substrate. The interaction strength is then reduced in two successive steps of 0.1 ns each until reaching the target value of $\varepsilon_{\text{Pt-water}} = 0.002$ eV. The total equilibration time is 0.5 ns, and atomic positions and velocities are recorded every 0.01 ns for subsequent analysis. To avoid unintended coalescence during equilibration, the water–water interaction between the two droplets is temporarily disabled throughout this stage.

(2) Coalescence and jumping stage

After equilibration, the water–water interactions are activated with parameters $\varepsilon_{\text{water-water}} = 0.16838$ eV and $\sigma_{\text{water-water}} = 2.8155$ Å. The system is then evolved in the microcanonical (NVE) ensemble for 0.3 ns to capture the coalescence and jumping dynamics. To resolve rapid events such as liquid bridge formation and droplet detachment, trajectory data are recorded at intervals of 0.001 ns. Two distinct motion modes are considered: (1) Translational mode: At the onset of the coalescence stage, a prescribed initial velocity v_0 is instantaneously assigned to the left droplet, after which the system evolves freely. (2) Rolling mode: The moving droplet is driven by a sustained uniform body force, which is continuously applied throughout the pre-contact movement process and the entire coalescence-jumping stage, even when the droplet undergoes severe morphological deformation and center-of-mass offset during coalescence. This force, with a pre-calibrated magnitude for each Weber number working condition, is uniformly applied to all water molecules of the target droplet to maintain its stable no-slip rolling state along the substrate. The force acts evenly on all atoms of the target droplet, and its action area does not need to be dynamically adjusted with droplet deformation.

For consistent comparison across different velocity conditions, the corresponding Weber number is determined by the liquid surface tension, density, characteristic length scale, and the imposed initial velocity. In this study, the Weber number is defined as $We = \rho v_0^2 r / \gamma$. The pairing between the prescribed v_0 values and their corresponding Weber numbers is summarized in Table 1. The dimensionless jumping velocity $v^* = v_{\text{ex}} / v_i$, where v_{ex} is the vertical departure velocity of the merged droplet at the jumping moment, $v_i = \gamma / (\rho r)$ is the inertial-capil-

TABLE 1
CORRESPONDENCE BETWEEN THE INITIAL VELOCITY v_0 AND THE WE USED IN THE PRESENT SIMULATIONS.

v_0 (m·s ⁻¹)	We
20	0.030181818
40	0.120727273
60	0.271636364
80	0.482909091
100	0.754545455
120	1.086545455
140	1.478909091
160	1.931636364
180	2.444727273

lary velocity scale, γ is the liquid–vapor surface tension of water, and $r = 5$ nm is the radius of the initial equal-sized droplets in this work

D. Model Validation

Given the inherent scale disparity between nanoscale simulations and macroscopic experiments, the reliability of the present model is assessed by examining the early-stage liquid bridge growth dynamics during droplet coalescence. Upon contact, a liquid bridge rapidly forms between the two droplets, and its characteristic radius increases with time. Under inertia-dominated conditions, the bridge expansion is expected to follow the classical inertial-capillary scaling law. The temporal evolution of the bridge radius obtained in this study exhibits clear agreement with this established scaling behavior, thereby validating the model's capability to accurately capture the interfacial dynamics during the initial stage of droplet coalescence.

III. RESULTS AND DISCUSSION

This section systematically examines the coalescence-induced jumping behavior of a moving droplet interacting with a stationary droplet under both translational and rolling modes. The analysis proceeds from morphological evolution to dynamic metrics and finally to energy partitioning, in order to establish a coherent link between liquid bridge growth, shape anisotropy, momentum generation, and energy conversion mechanisms.

Fig. 2 presents time-resolved morphological snapshots of coalescence-induced jumping between a moving droplet and a stationary droplet under different Weber numbers, including both top and side views. The dimensionless time $t^* = \Delta t / \tau$, where $\Delta t = t - t_a$, t is the physical time of the simulation process, t_a is the time at the moment of initial contact between the moving droplet and the stationary droplet, $\tau = (\rho r^3 / \gamma)^{1/2}$ is the inertial-capillary characteristic time. Three representative Weber numbers are considered, $We = 0.48$, 1.09, and 1.93, corresponding to panels Figs. 2(a)–2(c), respectively. At $We =$

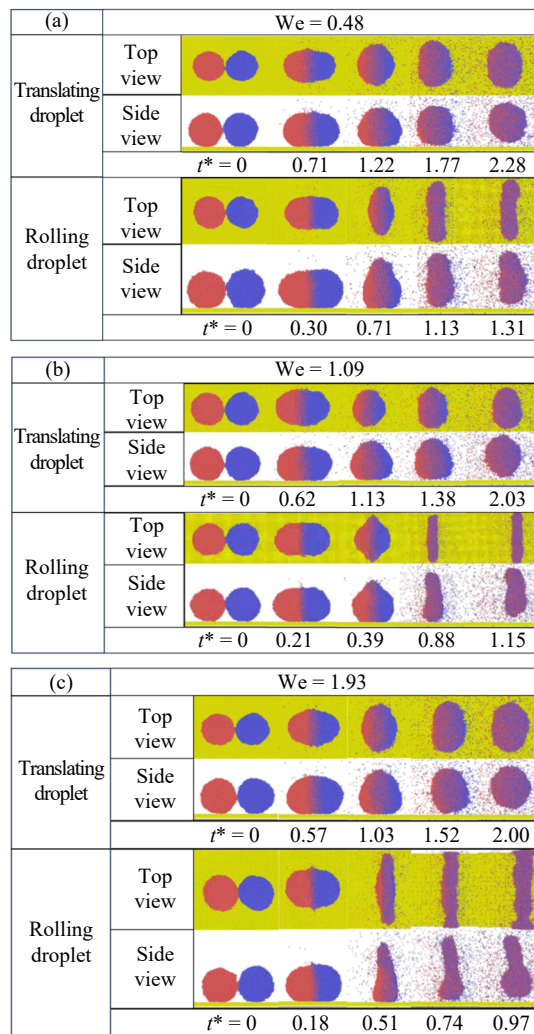


Fig. 2. Morphological evolution snapshots of coalescence-induced jumping between a moving droplet and a stationary droplet under different We: (a) We = 0.48, (b) We = 1.09, and (c) We = 1.93.

0.48, the two droplets establish contact and rapidly form an initial liquid bridge. Driven by surface tension, the bridge expands radially and gradually develops toward the substrate. Under the translational mode, the merged droplet exhibits a pronounced front-rear asymmetry along the direction of motion. After the initial bridge expansion, the droplet undergoes a relatively complete sequence of deformation and retraction, followed by the formation of a vertically elongated structure that ultimately detaches from the surface. In contrast, under the rolling mode at the same We, a slender vertical morphology emerges at an earlier stage. The merged droplet transitions more rapidly from in-plane stretching to axial contraction, and the formation of the off-surface structure occurs noticeably sooner than in the translational case.

As We increases to 1.09, the initial liquid bridge growth rate becomes faster, and the overall timescale of droplet evolution is compressed. Under the translational mode, a certain degree of in-plane stretching and morphological asymmetry remains

evident; however, the retraction stage proceeds more rapidly, and the merged droplet enters the vertical elongation phase at an earlier time. In contrast, under the rolling mode, an approximately axisymmetric vertical column forms within a shorter time interval. The downward development of the liquid bridge becomes more concentrated, and the side view clearly reveals enhanced vertical elongation and lifting characteristics. At We = 1.93, the formation and expansion of the liquid bridge are further accelerated. Compared with the We = 1.09 case, the translational mode exhibits a more pronounced forward shift in the overall evolution sequence, with the bridge expansion, retraction, and vertical lifting stages all completed within a shorter duration. The rolling mode similarly demonstrates rapid bridge growth and early establishment of a vertically elongated structure, with the merged droplet entering the detachment stage at an earlier time. Overall, increasing the Weber number progressively compresses the characteristic timescale of liquid bridge growth and morphological evolution. Across all We examined, the rolling mode consistently exhibits earlier development of vertically oriented structures. This difference in the timing of stage transitions provides the morphological basis for the subsequent quantitative analysis of velocity evolution and jumping time.

Fig. 3 illustrates the dependence of liquid bridge growth rate on We under translational and rolling modes. The bridge growth rate characterizes the expansion speed of the interfacial neck formed immediately after droplet contact. Physically, it reflects the intensity of curvature redistribution and fluid replenishment within the coalescence region, and thus serves as a key parameter linking the “coalescence dynamics timescale” to the subsequent detachment response. For the translational mode, the bridge growth rate exhibits relatively weak sensitivity to the Weber number. As We increases, the growth rate shows only a gradual variation or even approaches a plateau-like trend. This indicates that, within the present parameter range, simply increasing translational inertia does not continuously or significantly accelerate bridge expansion. The underlying reason is that translational momentum predominantly enhances in-plane stretching and asymmetric

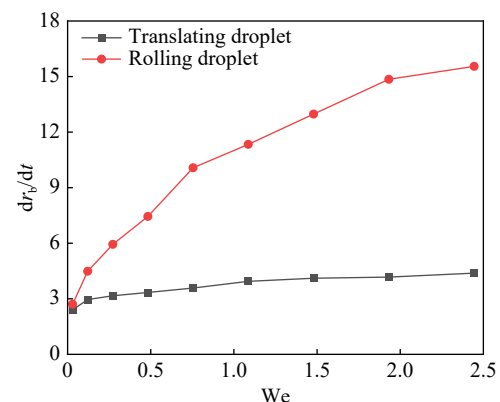


Fig. 3. Variation of the liquid bridge growth rate of We, comparing the translational and rolling modes.

deformation, whereas the effective radial mass supply and curvature-driven reconstruction within the bridge region do not scale proportionally with We . Consequently, the bridge growth rate remains largely governed by surface tension effects, leading to a comparatively weak response to increasing inertia.

In contrast, under the rolling mode, the liquid bridge growth rate exhibits a more pronounced increase with increasing We , particularly in the low-to-moderate We regime. This behavior suggests that the angular momentum and shear flow introduced by rolling motion modify the local flow structure in the neck region, thereby enhancing fluid replenishment during bridge expansion. As a result, the bridge growth process becomes more responsive to increases in inertial strength. As We continues to increase, the enhancement trend gradually weakens, indicating that the bridge expansion remains constrained by the intrinsic geometric reconstruction rate governed by surface tension. In other words, despite the additional rotational contribution, the interfacial dynamics cannot accelerate indefinitely due to the capillary-controlled upper limit of neck evolution. Therefore, rolling motion not only compresses the overall coalescence timescale but also directly intensifies the dynamic reconstruction of the interfacial neck. This distinction establishes the dynamical foundation for the subsequent divergence between translational and rolling modes in terms of jumping velocity, jumping time, and the efficiency of vertical momentum generation.

Fig. 4 presents the variation of the dimensionless jumping velocity with We under translational and rolling modes. For the translational case, the dimensionless departure velocity remains nearly constant over the investigated We range, exhibiting only minor fluctuations as We increases. This indicates that, within the present inertial regime, increasing the initial translational kinetic energy does not substantially enhance the final off-surface velocity. In other words, the jumping velocity does not scale linearly with We , but instead is constrained by the upper limit of releasable interfacial

energy. This result suggests that, at the nanoscale, surface tension continues to dominate the ultimate departure velocity in coalescence-induced jumping, while additional initial inertia primarily compresses the evolution timescale rather than increasing the magnitude of the final velocity.

In contrast, the rolling mode exhibits a distinctly different trend. As We increases, the dimensionless jumping velocity shows a clear upward tendency, particularly within the low-to-moderate We regime. This behavior implies that the angular momentum and internal shear flow introduced by rolling motion modify the efficiency of kinetic energy redistribution toward the vertical direction, enabling a portion of the initial inertial energy to be more effectively converted into off-surface momentum. Consequently, under rolling conditions, increasing the initial inertia not only shortens the morphological evolution timescale but also enhances the proportion of kinetic energy contributing to vertical momentum generation. At higher We , however, the growth rate of the departure velocity under rolling conditions begins to diminish. This suggests that, despite the presence of rotational coupling mechanisms, the system remains constrained by the combined effects of interfacial energy release and internal dissipation, leading to an upper bound in the attainable velocity scale. Overall, in the translational mode, the dimensionless jumping velocity is predominantly governed by surface tension and exhibits weak sensitivity to We . In contrast, under rolling motion, initial inertia participates in vertical momentum establishment through rotational coupling, resulting in an enhanced departure velocity within a certain We range. This distinction indicates that rolling motion alters not merely the characteristic timescale of coalescence, but more fundamentally the spatial partitioning of kinetic energy, thereby providing a crucial dynamical basis for the subsequent analysis of jumping time and energy conversion efficiency.

Fig. 5 illustrates the variation of the dimensionless jumping time with We for both translational and rolling modes. For the translational mode, the jumping time decreases monotonically

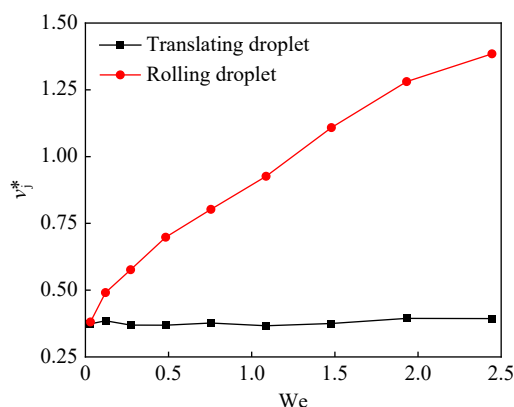


Fig. 4. Variation of the dimensionless jumping velocity of the merged droplet at the departure stage as a function of We , comparing the translational and rolling modes.

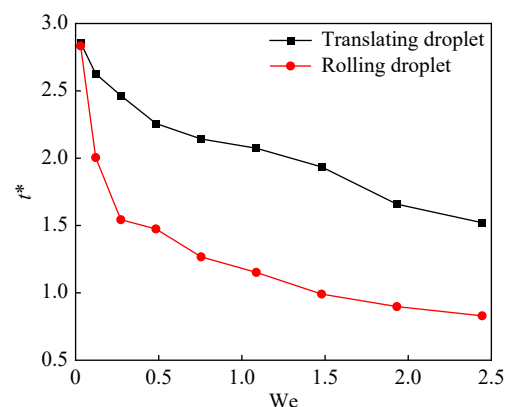


Fig. 5. Variation of the dimensionless jumping time of the merged droplet at the departure stage as a function of We , comparing the translational and rolling modes.

as We increases. Although the dimensionless departure velocity remains nearly constant, the total duration required for the system to complete the sequence of “contact–liquid bridge expansion–retraction–detachment” is significantly reduced. This indicates that increasing inertia primarily compresses the overall evolution timescale without substantially altering the final velocity magnitude. In other words, higher initial translational kinetic energy accelerates liquid bridge growth and morphological retraction, allowing the merged droplet to establish vertical momentum earlier, while surface tension continues to dictate the ultimate departure velocity scale. In contrast, the rolling mode exhibits consistently shorter jumping times than the corresponding translational cases across the entire We range. The jumping time also decreases with increasing We . More importantly, the temporal gap between the two modes persists throughout the investigated range. Rolling motion enables the system to enter the vertical elongation stage at an earlier moment, thereby shortening the time required for vertical momentum buildup. This temporal advantage becomes particularly pronounced in the moderate-to-high We regime.

When considered together with the dimensionless jumping velocity results, a clear distinction emerges. In the translational mode, enhanced inertia mainly accelerates the dynamic process while leaving the velocity ceiling unchanged. In contrast, under rolling motion, increased inertia not only shortens the evolution timescale but also, within a certain range, improves the efficiency of vertical momentum generation, leading to simultaneous optimization in both velocity and time. Overall, the jumping time exhibits stronger sensitivity to We than the jumping velocity, suggesting that within the present parameter regime, the system response manifests predominantly as process acceleration rather than reconstruction of the velocity scale. By modifying the initial momentum structure, rolling motion enables the merged droplet to complete bridge expansion and interfacial retraction more rapidly, thereby systematically advancing the detachment moment.

Fig. 6 presents the variation of the aspect ratio (defined as the ratio of horizontal extension to vertical height at the departure stage) with We under translational and rolling modes. The

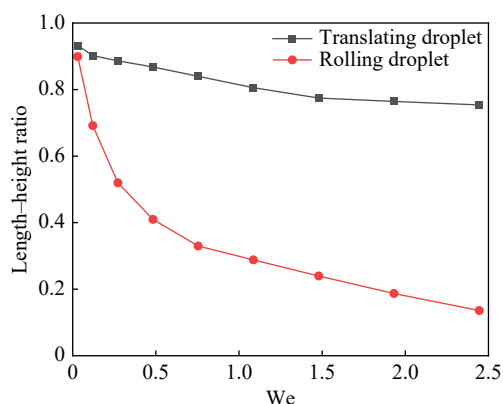


Fig. 6. Variation of the aspect ratio of the merged droplet at the departure stage as a function of We , comparing the translational and rolling modes.

aspect ratio serves as a geometric indicator of the relative deformation intensity in the horizontal and vertical directions and thus provides a quantitative measure of morphological anisotropy. For the translational mode, the aspect ratio exhibits only minor variation with increasing We . Although stronger inertia accelerates the overall evolution process, the degree of shape anisotropy does not increase significantly within the investigated We range. This suggests that translational inertia primarily influences the temporal progression of the process rather than altering the dominant deformation direction. During the retraction stage, the merged droplet retains pronounced in-plane stretching characteristics, while its vertical elongation remains comparatively limited. As a result, the sensitivity of the aspect ratio to We is weak.

In contrast, the rolling mode demonstrates a markedly different trend. As We increases, the aspect ratio decreases more noticeably, particularly in the low-to-moderate We regime. This indicates that rotational motion promotes the establishment of vertical structures, enabling the merged droplet to develop a more slender axial morphology. At the moment of contact, the rolling droplet carries angular momentum, and the internal flow field tends to form toroidal or spiral structures. Such flow patterns enhance axial focusing during the interfacial retraction stage, shifting the dominant deformation mode from in-plane stretching to vertical elongation. When We increases further, the reduction in aspect ratio under rolling conditions gradually levels off. This behavior suggests that, despite the presence of rotational coupling effects, geometric reconstruction of the droplet remains constrained by surface tension and volume conservation, leading to an intrinsic upper bound in achievable vertical elongation.

Overall, while the aspect ratio in the translational mode is relatively insensitive to We , the rolling mode exhibits a clear enhancement in vertical deformation with increasing inertia. This distinction indicates that rolling motion not only modifies the liquid bridge growth efficiency but also alters the dominant deformation pathway, allowing the system to enter a vertically elongation-dominated regime at an earlier stage. The observed geometric differences are consistent with the previously discussed trends in jumping velocity and jumping time, providing morphological evidence for the divergent dynamical mechanisms between translational and rolling modes.

Fig. 7(a) presents the energy comparison for the translational mode at different initial velocities v_0 . As expected, $E_{k,ini}$ increases nonlinearly with v_0 , following the quadratic dependence of kinetic energy on velocity. In contrast, the departure-stage $E_{k,x}$ exhibits an approximately linear increase with v_0 , indicating that stronger initial translational inertia leads to a larger fraction of horizontal momentum being retained at detachment. In other words, a greater portion of the input kinetic energy is inherited as translational motion along the original direction, rather than being fully dissipated through deformation and retraction during coalescence.

More importantly, $E_{k,y}$ shows only weak variation across the entire range of v_0 , remaining at a nearly constant level. This

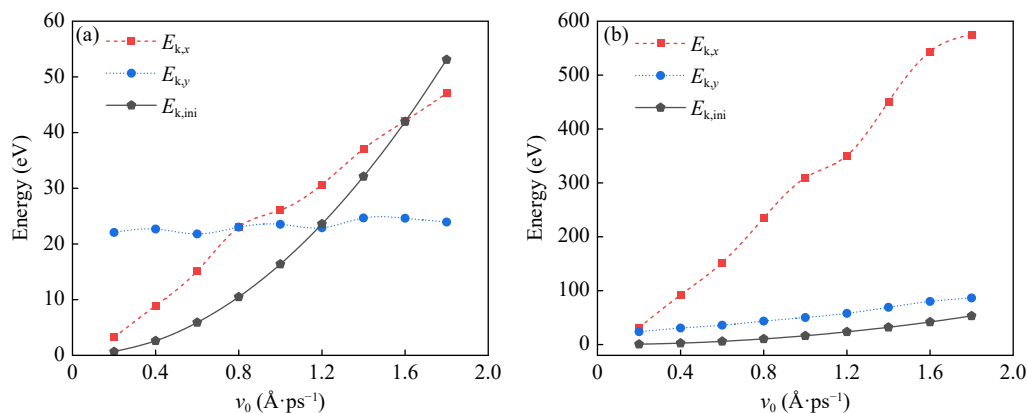


Fig. 7. Comparison of kinetic energy components of the merged droplet at the departure moment for $r = 5$ nm under different initial velocities v_0 : (a) translational mode and (b) rolling mode.

behavior implies that, under translational motion, the vertical jumping kinetic energy does not continuously increase with initial velocity but is instead constrained by an upper limit primarily governed by interfacial energy release and geometric recoil. Consequently, the ratio $E_{k,y}/E_{k,ini}$ decreases as v_0 increases, meaning that additional input kinetic energy is preferentially redistributed into horizontal motion, internal oscillations, or dissipative channels rather than contributing to vertical jumping. This observation is fully consistent with the earlier finding that the dimensionless jumping velocity in the translational mode is largely insensitive to We .

A crucial physical clarification is required here: even when $E_{k,ini} = 0$, both $E_{k,x}$ and $E_{k,y}$ remain finite at the departure moment. This does not violate energy conservation but instead reflects the conversion of excess surface energy ΔE_s released during coalescence into kinetic energy. When the two droplets merge and form a liquid bridge, the total interfacial area decreases, leading to the release of excess surface energy. During the subsequent retraction stage, this energy is converted into translational and oscillatory kinetic energy. Therefore, even in the absence of initial kinetic input, surface tension alone can generate both vertical and horizontal momentum, in agreement with classical theories of coalescence-induced jumping. Furthermore, in the low-velocity regime, it can be observed that $E_{k,x} + E_{k,y}$ at departure exceeds $E_{k,ini}$. This phenomenon is readily explained from an energy-source perspective. The initial kinetic energy constitutes only a portion of the total available energy, whereas the surface energy released during coalescence is often much larger than the initial kinetic energy at small v_0 . Consequently, the departure-stage kinetic energy is predominantly derived from surface energy conversion rather than inheritance of the initial kinetic input. When $E_{k,ini}$ is small, the surface-energy contribution dominates, leading to the apparent condition where the jumping kinetic energy exceeds the initial kinetic energy.

Fig. 7(b) shows the corresponding energy comparison under the rolling mode. The initial kinetic energy $E_{k,ini}$ again increases nonlinearly with v_0 , reflecting the quadratic velocity dependence. Similarly, $E_{k,x}$ increases monotonically with v_0 ,

indicating enhanced retention of horizontal momentum at departure, which is consistent with the translational case and confirming that initial inertia can be effectively inherited in the horizontal direction.

The key distinction lies in the vertical component $E_{k,y}$. Unlike the translational mode, where $E_{k,y}$ remains nearly insensitive to v_0 , the rolling mode exhibits a more pronounced increase in $E_{k,y}$ as v_0 increases. This indicates that the angular momentum and shear flow introduced by rolling do more than simply accelerate the process; they enhance the efficiency with which initial kinetic energy is redistributed into the vertical jumping channel. As a result, a larger fraction of the available energy is retained in a form conducive to detachment. In other words, the rolling configuration demonstrates a stronger capacity for vertical momentum buildup, directly supporting the earlier observation that the dimensionless jumping velocity increases with We under rolling conditions.

It is also important to interpret the cases where $E_{k,x}$ in the rolling mode significantly exceeds both $E_{k,ini}$ and $E_{k,y}$. This behavior can be understood in terms of energy redistribution mechanisms. At the moment of contact, a rolling droplet possesses not only translational kinetic energy but also angular momentum and shear-induced flow associated with substrate interaction. During coalescence, the released surface energy couples with rotational motion, causing a portion of the interfacial recoil energy to be preferentially projected along the horizontal direction. Because the rolling configuration inherently introduces directional bias, the recoil-driven momentum is not distributed axisymmetrically but instead concentrates along the original motion direction. This leads to a substantial enhancement of $E_{k,x}$ at departure. Despite the apparent amplification of horizontal kinetic energy, the total energy of the system remains conserved: the sum of the initial kinetic energy and the released surface energy equals the sum of translational kinetic energy, internal oscillatory energy, and viscous dissipation at departure. The fundamental difference of the rolling mode lies not in generating additional energy, but in altering the spatial partitioning of energy among different momentum channels.

Fig. 8(a) presents the energy conversion rate of the merged droplet at the departure moment under the translational mode for different initial velocities v_0 . The energy conversion rate is defined as the ratio between the translational kinetic energy at departure and the total available energy that can be converted during the coalescence process. Specifically, it can be expressed as

$$\varepsilon_x = \frac{E_{k,x}}{\Delta E_s + E_{k,ini}} \quad (2)$$

$$\varepsilon_y = \frac{E_{k,y}}{\Delta E_s + E_{k,ini}} \quad (3)$$

$$\varepsilon_{tot} = \frac{E_{k,x} + E_{k,y}}{\Delta E_s + E_{k,ini}} \quad (4)$$

From the observed trend, ε_y decreases overall with increasing initial velocity. Although the absolute magnitude of the vertical kinetic energy $E_{k,y}$ remains nearly constant, the denominator term $\Delta E_s + E_{k,ini}$ increases significantly as v_0 increases. As a result, the proportion of vertical kinetic energy relative to the total available energy is progressively diluted. This indicates that, under the translational mode, increasing the initial velocity does not substantially enhance the efficiency of vertical energy conversion. The vertical jumping capability therefore remains predominantly governed by surface tension rather than by the magnitude of imposed inertia. In contrast, ε_x exhibits a different behavior, showing an initial increase with v_0 followed by a plateau-like trend at higher velocities. As the initial velocity increases, a larger fraction of the input inertial energy is retained as horizontal momentum at departure, thereby increasing the contribution of horizontal kinetic energy to the total energy budget. However, in the higher-velocity regime, this growth gradually levels off. This saturation suggests the presence of enhanced dissipation and geometric constraints associated with interfacial reconstruction, which limit the continuous improvement of horizontal energy conversion efficiency.

Overall, the total energy conversion efficiency ε_{tot} exhibits

only limited variation across the investigated velocity range and may even display a slight decreasing trend. This behavior indicates that, under the translational mode, increasing the initial velocity primarily redistributes kinetic energy among spatial directions rather than substantially enhancing the overall fraction of energy that can be converted into translational kinetic energy at departure. The additional input kinetic energy is not fully transformed into effective departure motion; instead, a portion is dissipated through internal oscillations and viscous effects during the coalescence and retraction processes. This energy partitioning mechanism is consistent with the previously discussed trends in jumping velocity and jumping time, reinforcing the conclusion that inertia mainly accelerates the dynamics without fundamentally increasing the efficiency of energy conversion into detachment motion.

Fig. 8(b) presents the variation of the energy conversion rates at the departure moment under the rolling mode for different initial velocities v_0 . Under rolling conditions, $E_{k,y}$ increases with v_0 , in contrast to the nearly invariant behavior observed in the translational mode. This indicates that rolling motion enhances the establishment of vertical momentum. However, since the denominator term $\Delta E_s + E_{k,ini}$ grows more rapidly as v_0 increases, the vertical energy conversion rate ε_y still exhibits a monotonic decrease. Thus, although rolling improves the absolute vertical kinetic output, its proportion relative to the total available energy is progressively reduced as the initial energy input increases.

In contrast, ε_x displays a non-monotonic trend, first increasing and then decreasing with v_0 . In the low-to-moderate velocity regime, the angular momentum and shear flow induced by rolling promote directional concentration of momentum during interfacial retraction. This corresponds to the pronounced enhancement of $E_{k,x}$ observed in Fig. 7(b), reflecting effective inheritance and amplification of horizontal momentum, and leading to an increase in ε_x . As v_0 increases further, although $E_{k,x}$ may continue to rise in absolute magnitude, a larger fraction of the available energy is redistributed into internal oscil-

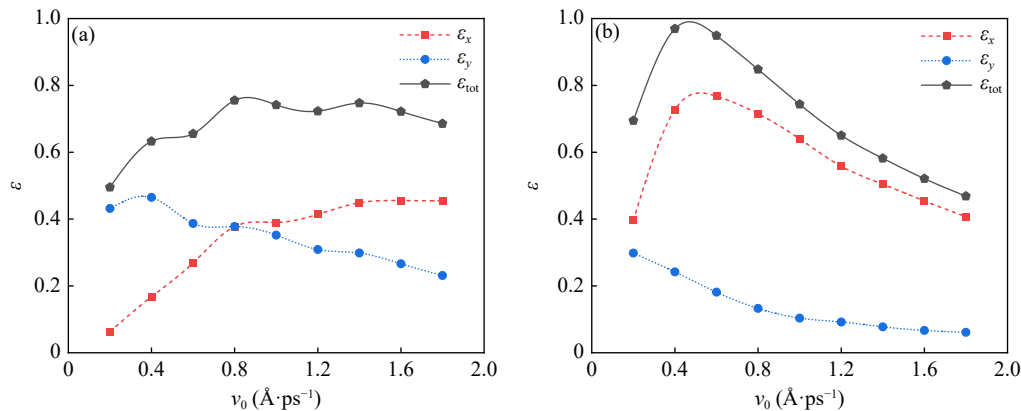


Fig. 8. Energy conversion rates of the merged droplet at the departure moment for $r = 5$ nm under different initial velocities v_0 . (a) translational mode and (b) rolling mode.

lations, localized shear, and substrate-related dissipation pathways. Consequently, the proportion of horizontal kinetic energy at departure decreases. As a combined result of these competing mechanisms, the total energy conversion rate ε_{tot} also exhibits a rise then decline behavior, indicating the existence of an intermediate velocity range in which rolling motion most effectively converts the available energy into translational kinetic energy at detachment.

IV. CONCLUSIONS

This study systematically investigated the coalescence-induced jumping behavior of translating and rolling nanodroplets on a superhydrophobic Pt substrate using molecular dynamics simulations, with emphasis on directional energy conversion and momentum redistribution mechanisms. The results show that under translational motion, increasing Weber number primarily shortens the coalescence and retraction timescale, while the dimensionless jumping velocity remains nearly invariant. The vertical kinetic energy is constrained by the upper limit of interfacial energy release, and additional input inertia is mainly redistributed into horizontal motion and dissipative pathways. Consequently, the vertical energy conversion efficiency decreases monotonically with increasing initial velocity.

In contrast, rolling motion significantly alters the momentum structure of the system. The absolute vertical kinetic energy increases with initial velocity, indicating enhanced vertical momentum establishment. However, the corresponding conversion efficiency still decreases due to rapid growth of total available energy. Meanwhile, horizontal and total energy conversion efficiencies exhibit a non-monotonic behavior, with an intermediate velocity range yielding the highest effective translational energy output. This demonstrates that rolling motion introduces a directional energy redistribution mechanism and an optimal inertial regime for energy utilization. Overall, rolling motion does not create additional energy but modifies the spatial partitioning of energy during interfacial reconstruction, leading to enhanced momentum transfer within a limited Weber number range. These findings provide nanoscale insights into phase-change-driven energy conversion and may contribute to the design of energy-efficient passive droplet removal strategies in thermal management and power systems.

DATA AVAILABILITY

Data will be made available on request.

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DECLARATION OF COMPETING INTEREST

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

AI USAGE STATEMENT

None.

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