

Small molecule propulsion driven by solvent-mediated ultrafast energy transfer from vibrations to self-translation

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Despite its interest, self-propulsion at the molecular scale remains an open challenge. In this work, we demonstrate through all-atom molecular dynamics simulations that vibrational excitation of the amphiphilic molecule nitromethane (CH_3NO_2) in water can lead to transient, directed propulsion. The excess vibrational energy is anisotropically transferred into the solvent, generating a mechanical instability that results in a short-lived net force between the solvent and the molecule. As a consequence, propulsion emerges along the axis of the molecule with speeds of up to $2.2 \text{ \AA/ps}$, which decay in subpicosecond timescales. Under periodic excitation, this effect is measurable as an enhancement of the translational diffusion coefficient. We show that, despite being sensitive to the solute-solvent interaction model, the propulsion mechanism introduced here is robust to changes in the force field employed to describe atomic interactions. Our findings highlight a propulsion mechanism that is solvent-mediated and externally tunable via vibrational excitation, providing insight into the principles governing active transport at the nanoscale.

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Self-propelling colloids have drawn considerable attention in recent years [1] as, in addition to the theoretical challenges they pose, they hold promise for a range of disruptive applications in fields such as microfluidics, medicine, or biotechnology. Downsizing them to the nanoscale is a central open scientific and technological challenge [2]. It might facilitate, for instance, artificial actuation on the subcellular scale and the scaling down of several technologies (such as lab-on-a-chip devices) [2].

Among the wide variety of microscale propulsion mechanisms, an inspiring case is self-thermophoresis, where propulsion results from the generation of local temperature gradients. It was experimentally observed for Janus (half-metallic/half-dielectric) microparticles [3]: Heating of the metallic section with a laser beam generates an asymmetric solvent temperature distribution and colloid propulsion (measured as a short-time mobility enhancement, prior to optical trapping). Propulsion induced by temperature gradients has also been studied numerically, although using mesoscopic or simplified models to describe the surrounding solvent [4–10].

The prospect of self-thermophoresis at the nanoscale appears bleak at the outset. While initially proposed as a possible explanation for the diffusion enhancement reported

for enzymes catalyzing exothermic reactions [11], it was later discarded on several grounds [11,12]. Arguably, three obstacles preclude any significant effect [13]: (1) The energies involved ($\approx 12 \text{ kJ/mol}$) are insufficient; (2) internal vibrations would quickly spread excess energy; and (3) fast propulsion direction randomization (from rapidly increasing rotational diffusion for smaller solutes). In fact, the very existence of a chemomechanical motility enhancement, experimentally reported for enzymes and small reactants, is currently the subject of intense debate [13].

However, at the molecular level, well-known vibrational and/or electronic excitation mechanisms [14] may involve significantly greater energies, on the order of hundreds of kJ/mol . Furthermore, specific energy pathways enable the efficient transfer of this excess molecular energy to the surrounding solvent in picosecond timescales [15]. Such mechanisms can be exploited to generate propulsion of asymmetric nanoparticles. In Ref. [16], we examined the use of electronic excitations that induce electric charge redistribution of fluorophores as a possible route to induce locomotion. Using a simplified model of a nanoparticle decorated with a standard (diatomic dipole) model [17] of a fluorophore, we showed that the solvation dynamics that follows periodic electronic excitation/de-excitation of the fluorophore results in enhanced diffusion of the nanoparticle/fluorophore complex in liquid water. The accompanying local temperature gradients were shown to be consistent with a molecular scale instance of self-thermophoresis. An important conclusion of Ref. [16] is that the energies typically available in electronic excitation radiative processes such as fluorescence are likely insufficient to produce significant propulsion at the nanoscale. However, other electronic excitation nonradiative processes exist for which the energies

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available are significantly larger, since the totality of the initial electronic excitation energy is funneled (on a subpicosecond timescale) into vibrational energy on the ground electronic state. This is a ubiquitous process in nature, key for the photostability of DNA [18], and common for small molecules [19].

In this work, we focus on the possibility of propulsion induced by the vibrational excitations resulting from such internal conversion processes. In particular, we show that fast relaxation of specific high-energy vibrational excitations of nitromethane (NM, CH_3NO_2) is capable of inducing directed propulsion in liquid water. Several distinct aspects may be worth highlighting before proceeding: (1) nitromethane is one of the smallest molecules (seven atoms) for which one might expect that its anisotropy (i.e., its amphiphilic character, with a hydrophilic nitro group, NO_2 , and a hydrophobic methyl group, CH_3) might be exploited; (2) the solvent considered is water, of evident biological relevance but characterized by a high viscosity (chemomechanical propulsion has only been computationally shown to occur for solvents with viscosities orders of magnitude smaller [13,20]); (3) the models used consist, for both solvent and solute, of state-of-the-art all-atom force fields, i.e., first principles generated potentials, with no recourse to effective or coarse-grained dynamics; (4) energy fluxes, temperature gradients, and the resulting propulsion are emergent properties; none of them is initially fixed or sustained artificially; and (5) the excitation process stems from external radiation; it could thus be turned on and off at will, being biologically friendly. In the recent work [21], we investigated the energy relaxation dynamics of vibrationally excited nitromethane immersed in liquid water, among other environments. The core result was a marked anisotropic transfer of the initial vibrational energy (200 kJ/mol) to the surrounding water molecules, with most of it being transferred from the nitro group (as expected due to its stronger coupling with water), within ≈ 1 ps. These features suggested that, according to the arguments previously discussed, diffusion enhancement may result.

We consider here a system made of 1 NM and 512 water molecules, placed in a cubic box of side $24.8 \text{ \AA}$ to attain a density of 1.0034 g/cm^3 and periodic boundary conditions [21] (we refer to Sec. I in the Supplemental Material [22] for a summary of models and methods, and to Ref. [21] for a fuller account). Initial configurations are extracted (every 1 ps) from a long equilibrium trajectory at fixed temperature (300 K). After 1 ps of NVE dynamics (microcanonical ensemble), for each configuration an excess energy of 200 kJ/mol is deposited on a specific mode as kinetic energy in the noninertial Eckart frame [21,23]. These starting configurations are further evolved with NVE dynamics for an additional 2–4 ps, depending on the magnitudes measured. The reported results correspond to averages of at least 500 independent trajectories (for each mode). All molecular dynamics simulations were performed using LAMMPS [24].

Several intramolecular force fields for nitromethane were shown to be comparably satisfactory when benchmarked against single-molecule *ab initio* calculations (for both vibrational spectra and nuclear dynamics) [21]. This turns out not to be the case for intermolecular interactions. A marked sensitivity of the dynamics of vibrationally excited

NM on the force field exists, reminiscent of a similar behavior for thermophoresis (to the point that it is considered one of the most exacting tests of a force field [25]). We have therefore chosen to simultaneously consider the two state-of-the-art models available (both being excellent and almost indistinguishable for neat liquid NM [26]; see Sec. I in the Supplemental Material [22] for a detailed assessment): (1) the Sorescu-Rice-Thompson (SRT) model [26,27] and (2) the Alper-Abu-Awad-Politzer (AAP) model [28]. Water molecules were described using the extended simple point charge (SPC/E) water model [29]. Considering that NM has 15 vibrational modes, in order to better frame the results we note that for both SRT and AAP two distinct groups of modes can be distinguished [21] (see Sec. II in the Supplemental Material [22]): (1) fast relaxation modes, associated with low-frequency motions mostly located on the nitro group and (2) slow relaxation modes (with high frequency and relaxation times one order of magnitude larger), mostly associated with distortions of the methyl group. Only a subset within the first subgroup has the ability to induce propulsion.

The impact of each mode's vibrational relaxation on propulsion, if any, has been monitored through the average time dependence of NM's center-of-mass (CoM) velocity projected onto the molecular axis (C–N bond). Figure 1 displays the core results of the present work. For AAP, propulsion emerges for two modes (with propulsion velocity in the nitrogen-to-carbon direction): M2 (480 cm^{-1} , nitro group rocking [21]), with the largest propulsion peak speed ($v_{\text{max}} \approx 2.2 \text{ \AA/ps}$), M5 (918 cm^{-1} , combination of nitro bend and C–N stretching), with half the maximum speed ($\approx 0.82 \text{ \AA/ps}$). As for the SRT model, again two modes give rise to propulsion: M2 as well, with now a lower peak ($v_{\text{max}} \approx 0.30 \text{ \AA/ps}$), and M4 (480 cm^{-1} , nitro group wagging [21]), with *negative* (from C to N) propulsion velocity ($v_{\text{max}} \approx 0.77 \text{ \AA/ps}$). No other mode displays any noticeable propulsion effect. We note that the differences between models can be traced down to the Lennard-Jones diameters for NM's interaction sites (see Sec. I in the Supplemental Material [22]). Several additional features stand out: (1) Propulsion is rare, occurring for $\approx 10\%$ of the modes; (2) both propulsion directions are found (a common feature for thermophoresis [20,30], with thermophilic and thermophobic motions); (3) propulsion velocities are time varying and short-lived; and (4) in contrast, peak speeds ($\leq 2 \times 10^8 \text{ \mu m/s}$) are six orders of magnitude larger than the typical *constant* speeds ($\approx 100 \text{ \mu m/s}$) of natural/artificial microswimmers [2], although comparable to the CoM equilibrium thermal speed.

Given these provisos, an immediate question that arises is whether a periodic energy input into the vibrational modes that generate propulsion can lead to an observable diffusion enhancement. To address this issue, we have performed NVE simulations in which 200 kJ/mol is deposited in a given normal mode of nitromethane every $\Delta t = 5 \text{ ps}$ (a time lapse in which full vibrational relaxation occurs). Since a substantial amount of energy is inserted over the 200 ps length simulations, 8000 water molecules are now used so that temperature raises by just $\approx 12 \text{ K}$ (from the initial equilibrium temperature of 300 K). Although diffusion is only feebly dependent on temperature, and this increase should have no noticeable impact, a separate NVE control simulation (with no excitations)

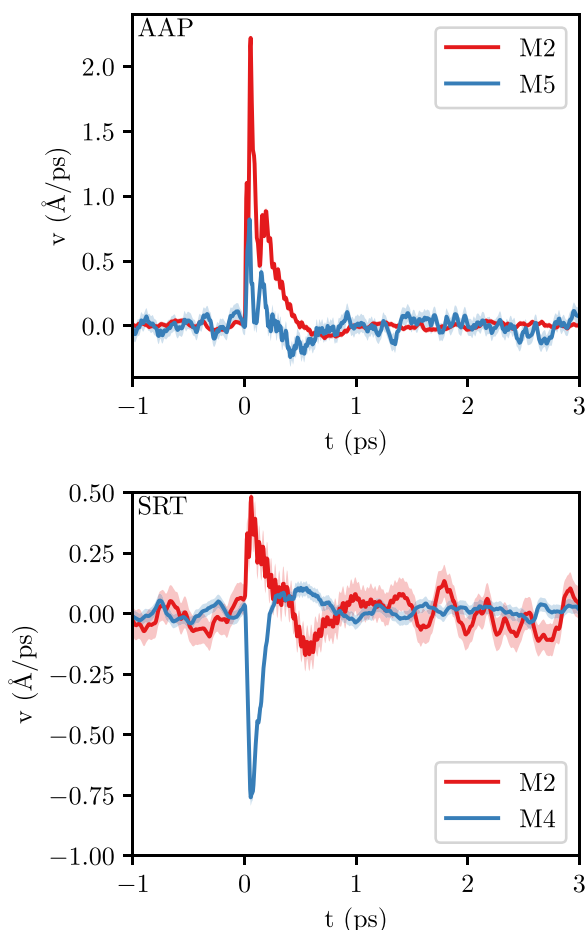


FIG. 1. Nitromethane's center-of-mass (average) velocity projected onto the axis defined by the C-N bond (positive direction defined from N to C), as 200 kJ/mol excess energy is deposited at $t = 0$. Top: AAP model with energy deposited in normal modes M2 (red line) and M5 (blue line). Bottom: SRT model with energy deposited in modes M2 (red) and M4 (blue).

is performed at $\langle T \rangle = 310$ K (the maximum *final* temperature for the nonequilibrium trajectories is 312 K). Results averaged over 500 independent trajectories are shown in Fig. 2 for periodic excitations of M2 and M5 (AAP model; see Sec. III in the Supplemental Material [22] for SRT). The diffusion coefficients are, respectively, 26% and 13% higher than those for the equilibrium case. We conclude that the large propulsion velocity compensates for speed fluctuations and fast rotational diffusion. This enhancement of the diffusivity can be understood, as a first approximation, by using recent analytical results for the active Brownian particle model subject to periodic pulses [31] (see Sec. IV in the Supplemental Material [22]).

Having thus demonstrated the actuality of propulsion and its significant effects on the diffusive dynamics of NM, the all-atom nature of our simulations allows for a detailed analysis down to the atomic scale. Figure 3 displays the total force on each NM atom (projected on the C-N axis of propulsion), with $t = 0$ denoting the time at which M2 (AAP model; see Sec. V in the Supplemental Material [22] for other cases) is excited. Before excitation (negative times), water molecules on the

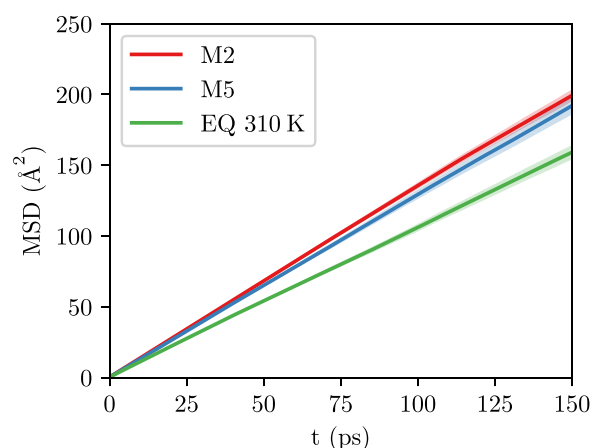


FIG. 2. Nitromethane's center-of-mass mean square displacement (MSD) for the AAP model under repeated excitation of vibrational modes M2 (red) and M5 (blue), as well as for the equilibrium case at $\langle T \rangle = 310$ K (green).

nitro end *pull* the oxygen atoms, which is mostly compensated by an opposite pull on the nitrogen atom, a dynamic equilibrium stemming from the strong Coulomb forces present. In contrast, forces on the methyl group are comparatively minor and constant along the whole process, in line with its hydrophobic nature. Upon excitation, the force on the oxygen atoms displays strong oscillations, momentarily vanishing at times, while the force on nitrogen decreases without any noticeable oscillations. This imbalance generates peaks of the total force of ≈ 60 kJ/(mol Å), in the N to C direction.

Analysis of the evolution of NM's first hydration shell suggests a mechanistic origin for the force imbalance that generates its propulsion. We observe that vibrational excitation of NM is accompanied by significant fluctuations in the hydration number around the nitro and methyl groups, pointing to a disruption of the hydration structure with respect to equilibrium. We note that propulsion consistently occurs from the moiety exhibiting greater disruption of the solvation

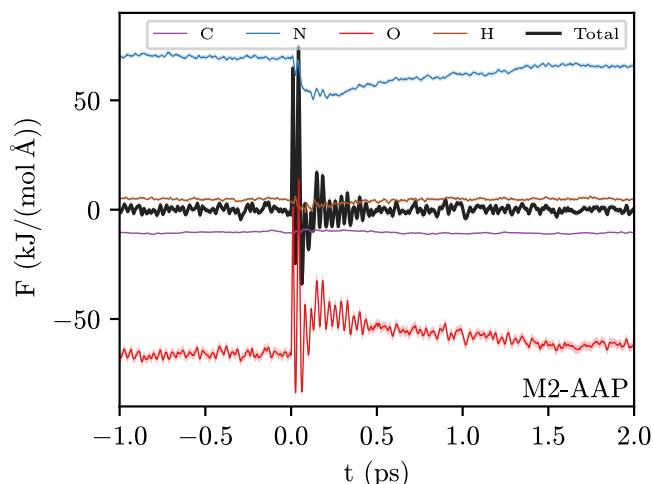


FIG. 3. Per-atom force projected onto the axis defined by the C-N bond after an energy deposit of 200 kJ/mol on mode M2 at $t = 0$ (AAP model).

structure toward the one with comparatively lesser change, a trend observed in both thermophobic and thermophilic regimes (see Sec. VI in the Supplemental Material [22]). This effect, together with the evolution of forces acting on the nitromethane atoms shown in Fig. 3, identifies the origin of the propulsion mechanism as a transient breaking of mechanical equilibrium caused by a disturbance of the hydrogen-bond network of hydration water molecules.

The efficiency of propulsion, i.e., the fraction of the initial excess energy channeled into self-translation, can be obtained by monitoring the evolution of the CoM kinetic energy change (a simple instance of the energy flux methodology [32], see Sec. VII in the Supplemental Material [22]). We note that this energy will reach a maximum before eventually returning to equilibrium. The maximum energy transferred (for M2, AAP model) is 2.8 kJ/mol, i.e., an efficiency of 1.4% (see Sec. VII in the Supplemental Material [22]). The underlying cause for this, in principle, low value can be traced to the lack of a direct coupling between CoM motion and internal dynamics. Any energy transfer from internal energy to self-translation is indirect and necessarily mediated by the water solvent. The efficiency obtained may be better appraised if compared, for instance, with the case of water bend relaxation: Energy transferred into self-translation, if any, is here indistinguishable from thermal noise, while approximately 50% of the initial excess energy is directly transferred into self-rotation (due to a direct Fermi-type rotation-vibration coupling [33]). We thus conclude that (indirect) transfer from M2 into self-translation for NM is actually substantial and that self-rotation excitation should always be expected (Sec. VII in the Supplemental Material [22] contains a summary of the formulas used for computation of power/work, together with the time-dependent behavior that results for both M2-AAP and M4-SRT).

Considering its indirect solvent-mediated origin, the ultrafast character of the total force is remarkable (Fig. 3). A somewhat puzzling aspect is that its associated timescale appears to be shorter than that of the propulsion velocity to which it gives rise, while no inertia is to be expected at this scale. The all-atom nature of the present calculation is revealing in this connection. If the total force is split into the contributions of nitrogen and oxygen(s), their return to equilibrium (Fig. 3) is considerably slower and compatible with that of the propulsion velocity. Moreover, they pull in opposite directions, being almost balanced. This suggests that a more intuitive understanding might be obtained in terms of a balance between *friction* and *propulsion* force, F_{prop} (as opposed to the *total* force, F_{total} , discussed so far). Given the short timescales involved, we resort to the generalized Langevin equation for translational motion along the C–N axis:

$$F_{\text{total}} = m\ddot{x} = F_{\text{prop}} - m \int_0^t M(t - \tau)v(\tau)d\tau + R(t), \quad (1)$$

which, when averaged over realizations, yields the average propulsion force in terms of the known total force and friction: $\langle F_{\text{prop}}(t) \rangle = \langle F_{\text{total}} \rangle + m \int_0^t M(t - \tau)\langle v(\tau) \rangle d\tau \equiv \langle F_{\text{total}}(t) \rangle + \langle F_{\text{friction}}(t) \rangle$, where the friction kernel ($M(t)$) can be simply obtained from the equilibrium velocity time correlation function (see Sec. VIII in the Supplemental Material [22]). Results are displayed in Fig. 4. They make evident

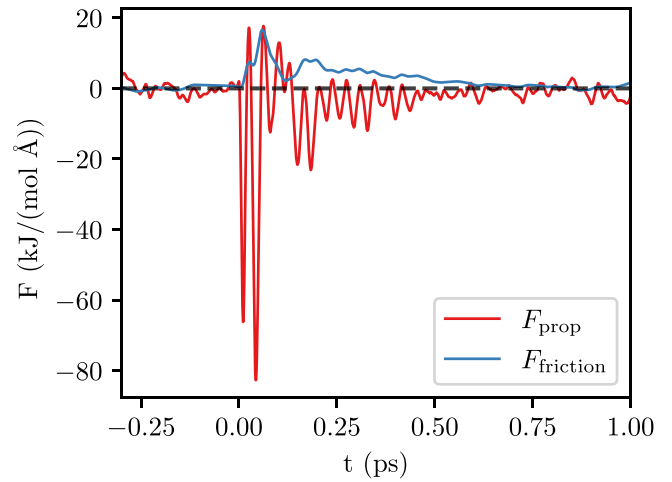


FIG. 4. Propulsion (red) and friction (blue) forces projected onto the axis of propulsion after excitation at $t = 0$ of mode M2 using the AAP model. A dashed horizontal line indicates $F = 0$ as a guide to the eye.

that both the propulsion force and friction are characterized by countering long-time tails that (as time progresses) balance each other. This so far hidden feature explains the longer lifetime of the propulsion velocity when compared with the total force.

Finally, we address the issue of whether NM propulsion might be considered a molecular-scale instance of self-thermophoresis (the phenomenological propulsion class that inspired this work and Ref. [16]). In Ref. [21], it was shown (Figs. 10 and 11) that the spatial distribution of the energy fluxes (work) from the highly excited NM into the immediate solvent is nonhomogeneous. This necessarily translates into an uneven temperature distribution, as displayed in Fig. 5 (for M2 AAP), where time-dependent temperatures on the nitro and methyl sides are compared (in Sec. IX in the

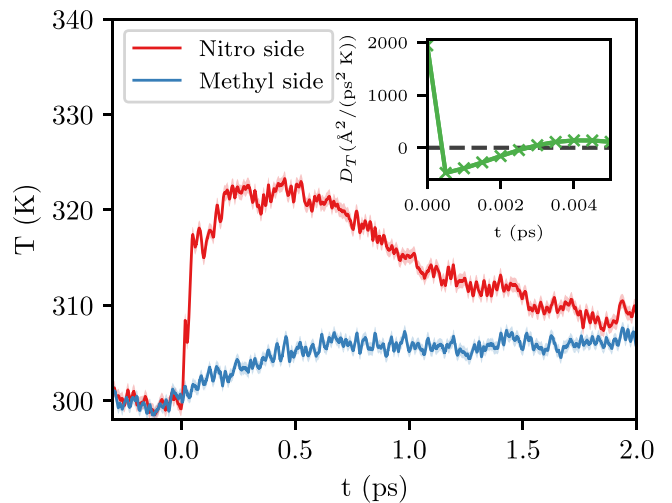


FIG. 5. Temperature on both sides of the nitromethane molecule after an excitation at $t = 0$ on mode M2 using the AAP model. Inset shows the time-dependent thermal diffusion coefficient, $D_T(t)$, see Sec. IX in the Supplemental Material [22] for details.

Supplemental Material [22], a similar result is displayed for M4-SRT). For a constant temperature gradient, thermophoresis is described by the constitutive relation $v = -D_T \nabla T$, which defines the thermal diffusion coefficient D_T [30]. Here, the temperature dependent gradient is characterized by a lifetime comparable to that of the propulsion velocity, which suggests that the generalization to frequency space might apply: $v(\omega) = -D_T(\omega) \nabla T(\omega)$. Inversion of this relation provides an estimate of the time-dependent thermal diffusion coefficient $D_T(t)$ (see Sec. IX in the Supplemental Material [22]), which is shown in Fig. 5 (inset) for the M2 excitation using the AAP model.

A reasonable delta-like thermal diffusion function is obtained, consistent with an almost direct proportionality between temperature gradient and velocity. When integrated, it yields $D_T \approx 1 \times 10^{-6} \text{ m}^2 \text{ K/s}$, some four orders of magnitude larger than the range characteristic of micrometric particles [30], in line with the much larger propulsion velocities previously discussed. While the high correlation between temperature gradient and propulsion seems to be compatible with thermophoresis, it should be noticed that here the mere existence of a thermal gradient is a necessary but not sufficient condition for propulsion, as this gradient must have been created by a particular vibrational mode. For colloids, D_T is highly sensitive to a myriad of factors [25,34] (total mass, mass distribution, moment of inertia, surface groups, etc.) and can even reverse its sign with temperature. Therefore, should the present mechanism be ascribed to the thermophoretic class, it would add an additional layer of complexity to this evasive phenomenon.

We conclude by highlighting the subnanometer size of the propelling molecule and the propulsion mechanism stud-

ied here, which can help open directions in the search for nanoscale propulsion. In particular, we provide a quantitative estimate of the excess energy and relaxation times that enable propulsion at the molecular scale. Our work introduces the potential of molecular excitation processes as a means of transferring substantial energies at the nanoscale. In this connection, one could imagine that photochemical reactions could also provide a convenient ground when looking for small reactant propulsion. Finally, it is important to highlight that in this work we employ a complete all-atom model of the system using well-established interaction potentials, where propulsion—or external gradients driving locomotion—are not imposed externally but arises naturally from solvent relaxation mechanisms. In contrast to the well-known challenges of capturing a detailed picture of thermophoresis in liquids [34], this approach enables a molecular-level understanding of a related phenomenon.

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Data availability. Data and code supporting this study are available in the public repository in Ref. [39].

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