Title:	Orientational dynamics of a heated Janus particle
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Abstract:	Using large scale molecular dynamics simulations, we study the orientational dynamics of a heated Janus particle which exhibits self-propulsion. The asymmetry in the microscopic interaction of the colloid with the solvent is implemented by choosing different wetting parameters for the two halves of the sphere. This choice leads to a different microscopic Kapitza resistance across the solid-fluid boundary of the two halves of the sphere, and consequently a gradient in temperature is created across the poles of the sphere. It is this self-created temperature gradient which leads to a self-propulsion along the direction of the symmetry axis. In this article, we look at the orientational dynamics of such a system, as well as the subsequent enhancement of the translational diffusivity of the heated Janus colloid at late times. The orientational correlation of the symmetry axis is measured from the simulation and provides a direct access to the rotational diffusion constant. The heating leads to an increase in the rotational diffusivity of the colloid. We quantify this increase in rotational diffusion Dr against the temperature difference δT ≡ T(R, 0) − T(R, π) across the poles of the Janus sphere as well as the average surface temperature difference ΔT ≡ T(R) − T(∞) from the ambient fluid. Since the rotational diffusion is determined by the complete flow field in the solvent, we illustrate that comparing Dr against δT is misleading and is better quantified when compared against ΔT. The later quantification results in a data collapse for different choices of the microscopic interaction. The average propulsion velocity is also measured for different choices of the wetting parameter. The directionality of self-propulsion changes depending on the microscopic interaction. We show that whenever the attractive interaction of the colloid with the solvent is switched off, the phoretic mobility changes sign. Furthermore, the propulsion velocity is zero for heating below a certain threshold value. This is also corroborated by the probability distribution of the angle between the displacement vector Δr(t) ≡ r(t) − r(0) and the symmetry axis. Finally, we combine the measured propulsion velocity and the rotational diffusion time τr = 1/2Dr to estimate the enhancement in the long time diffusion coefficient of the particle.
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