

Abstract Submitted
for the DFD14 Meeting of
The American Physical Society

Translational and rotational diffusion of a single Janus nanoparticle in an explicit solvent¹ ALI KHARAZMI, Michigan State University, NIKOLAI PRIEZJEV, Wright State University — Molecular dynamics simulations are carried out to study the translational and rotational diffusion of a Janus particle in a Lennard-Jones fluid. We consider a spherical particle with two hemispheres of different wettability. The analysis of the particle dynamics is based on the time-dependent orientation tensor, particle displacement, as well as the translational and angular velocity autocorrelation functions. We show that both translational and rotational diffusion coefficients increase with decreasing surface energy at the nonwetting hemisphere. It was found that in contrast to uniform particles, the nonwetting hemisphere of the Janus particle rotates in the direction of the displacement vector during the rotational relaxation time.

¹NSF CBET-1033662

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Date submitted: 30 Jul 2014

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