

Abstract Submitted
for the DFD16 Meeting of
The American Physical Society

Molecular dynamics simulations of the rotational and translational diffusion of a Janus rod-shaped nanoparticle. ALI KHARAZMI, Michigan State Univ, NIKOLAI PRIEZJEV, Wright State University — We investigate the diffusion of a Janus nanoparticle immersed in a dense Lennard-Jones fluid using molecular dynamic simulations. In particular we consider a rod-shaped particle with different surface wettability on each half-side of the particle and analyze the mean square displacement and the translational and rotational velocity autocorrelation functions. It is found that diffusion is enhanced when the wettability contrast is high and the local slip length on the nonwetting side is relatively large. We also examine the time evolution of the orientation tensor and correlate it with the particle displacement. These results are compared with our previously published results on diffusive dynamics of a Janus sphere with two hemispheres of different wettability.

Ali Kharazmi
Michigan State Univ

Date submitted: 28 Jul 2016

Electronic form version 1.4