Abstract Submitted
for the DFD13 Meeting of
The American Physical Society

Correlation between translational and rotational diffusion of a Janus nanoparticle in explicit solvent: A molecular dynamics simulation study ALI KHARAZMI, Michigan State University, NIKOLAI PRIEZJEV, Wright State University — Molecular dynamics simulations are used to study the diffusion of a single Janus particle immersed in a Lennard-Jones fluid. We consider a spherical particle with two hemispheres of different wettability. We analyzed the time dependence of the orientation tensor, particle displacement, and translational and rotational velocity autocorrelation functions. It was found that both translational and rotational diffusion coefficients increase with decreasing surface energy of the nonwetting hemisphere. We also observed that in contrast to homogeneous particles, the nonwetting hemisphere of the Janus particle tends to rotate in the direction of the displacement vector during the rotational relaxation time.

Nikolai Priezjev
Wright State University

Date submitted: 02 Aug 2013 Electronic form version 1.4