Abstract Submitted
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Molecular Dynamics Study of Janus Particle Aggregates in Shear Flows SINA SAFAEI, The MacDiarmid Institute for Advanced Materials and Nanotechnology, Department of Physics, University of Auckland, New Zealand, SHAUN HENDY, Te Pūnaha Matatini, Department of Physics, University of Auckland, New Zealand, GEOFF WILLMOTT, The MacDiarmid Institute for Advanced Materials and Nanotechnology, Departments of Physics and Chemistry, University of Auckland, New Zealand — Janus nanoparticles have attracted much interest recently because of the way that they interact with each other to self-assemble into complex nanostructures. Theoretical studies indicate that amphiphilic Janus nanoparticles experience a torque in fluids due to their slip-asymmetric boundary conditions, and our molecular dynamics simulations have verified this [1]. As a result, Janus self-assembled nanostructures could be unstable in fluid flows. Most previous molecular dynamics studies have used soft-sphere potentials to study Janus nanoparticle self-assembly processes, but such methods dont capture the effect of slip boundary conditions at the spheres surfaces. We have studied thermal- and shear-induced break-up of Janus and homogeneous hydrophobic dimers in a fluid using a hard-sphere potential [2]. We will present our latest results investigating the possible mechanisms which lead to increased break-up probability, and propose a theoretical expression for all effective parameters contributing to the breakup rate. Overall, the Janus dimers are less stable than hydrophobic dimers, and their stability depends on the slip length at the spheres surfaces. [1] Safaei, Sina, et al. Soft Matter (2019). [2] Safaei, Sina, Shaun C. Hendy, and Geoff R. Willmott. Soft Matter (2020).

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