

Abstract Submitted
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Deviations from Jefferys theory in the dynamics of atomically-thin sheet-like molecules in shear flow¹ SIMON GRAVELLE, CATHERINE KAMAL, School of Engineering and Material Science, Queen Mary University of London, London, United Kingdom, LORENZO BOTTO, Process and Energy Department, 3ME Faculty of Mechanical, Maritime and Materials Engineering, TU Delft, Delft, The Netherlands, BOTTO RESEARCH GROUP TEAM — The rotational dynamics of anisotropic colloidal particles in shear flow is well known for objects satisfying the hydrodynamic no-slip boundary condition. Jeffery’s theory predicts that, at high Pclet numbers, a no-slip particle rotates continuously about one of its axis. However, our recent results for particles constrained to move in the flow-gradient plane suggest that Jeffery’s theory fails to predict the rotational dynamics in the case of large hydrodynamic slip. For a slip length larger than its thickness, a particle is predicted to find an equilibrium orientation at a small angle with the flow [Kamal et al., Nat. Commun., 11, 2020]. The dynamics in shear flow of atomically-thin molecules must therefore be reconsidered. Using molecular dynamics, we study the flow dynamics of aromatic molecules, whose features are similar to graphene nanosheets. We show that aromatic molecules align in the direction of the shear flow with a constant average orientation angle, and that this alignment is due to hydrodynamic slip, in keeping with the theory. In the case of a single aromatic molecule, the trend of average molecular orientation for varying Pclet numbers is captured by a simplified Fokker-Planck equation. Multiple particle simulations illustrate the importance of clustering.

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