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Continuum and Molecular Dynamics Studies On the Diffusiophoretic Motion NIMA SHARIFI-MOOD, JOEL KOPLIK, CHARLES MAL-DARELLI, the City College of New York & Levich Institute — The self-propulsion of micron or sub-micron objects has a number of applications as miniaturized motors. One method for particle self propulsion is to utilize a surface chemical reaction on one part of the particle surface to create concentration gradients of solutes across the particle. These gradients drive a diffusiophoretic motion due to unbalanced (van der Waals) attractions between the particle and the solutes and solvent within an intermolecular length scale (L, 10-100 nm) of the particle surface. Prior continuum studies assume the interaction creates a local slip velocity at the particle surface, and find the terminal velocity U of spherical particles to be independent of the radius a. We provide numerical solutions for U which account directly for the solute transport and flow within L, and matched asymptotic solutions as L/a tends to zero. The leading order expression for U is independent of a, but U decreases with the particle radius for L/a greater than .01. Molecular dynamics simulation is also undertaken using Lennard-Jones potentials to provide a more complete picture of nanoscale propulsion.

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