Abstract Submitted
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Molecular Dynamics of Reaction-Driven, Diffusiophoretic, Colloid Self-Propulsion NIMA SHARIFI-MOOD, Levich Institute, Department of Chemical Engineering, City College of New York, JOEL KOPLIK[1], Department of Physics, City College of New York, CHARLES MALDARELLI, Levich Instiute, Department of Chemical Engineering, City College of New York — Chemical-mechanical transduction mechanisms which can actuate the movement of colloids through pathways in liquids are highly sought after as engines to propel miniaturized micro and nanobots. One mechanism involves harnessing van der Waals attractive forces between the colloid and solute molecules. Self propulsion can be achieved by arranging for the solute to react on one face of the colloid, creating an asymmetric distribution which can propel the particle. We use molecular dynamics calculations to elucidate this propulsion for nanocolloids. The calculations assume Lennard-Jones interactions between the colloid (modelled as a rigid cluster of atoms), solvent atoms and solute atoms which react with the colloid atoms on one face of the cluster. The solute reacts when localized within the attractive landscape of the cluster atoms and is converted for simplicity to solvent. Quantitative calculations of the diffusiophoretic velocity demonstrate the interplay of Brownian rotation and diffusiophoretic propulsion, the dependence of the nano-colloid velocity on its radius and an agreement with a continuum model which therefore allows a description of the phenomena for propulsion of objects in size and over trajectories from the nanometer to the micron scale.

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