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Chemically Powered Nanomotors

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Molecular motors play important roles in transport in biological systems. These molecular machines are powered by chemical energy and operate in the regime of low Reynolds number hydrodynamics. Recently a class of simple inorganic molecular motors has been constructed and studied experimentally [1,2]. These motors are bimetallic rods, one end of which is chemically active. The talk will describe simple mesoscopic models for the motion of such nanomotors. The motor consists of two linked spheres, one of which catalyzes the conversion between two chemical species. The chemical species interact differently with the the two spheres in the dimer. The nano-dimer motor is solvated by a molecules treated at a mesoscopic level whose evolution is governed by multi-particle collision dynamics. The dynamics conserves mass, momentum and energy so that coupling between the nanomotor and the hydrodynamic modes of the solvent is treated correctly. The simulations allow one to explore the mechanisms of the chemically powered motion and the effects of fluctuations on the motor dynamics.

[1] W. F. Paxton, et al., "Catalytic Nanomotors: Autonomous Movement of Striped Nanorods," J. Am. Chem. Soc. (JACS), 126 (41), 13424 (2004).
[2] S. Fournier-Bidoz, et al. "Synthetic Self-Propelled Nanorotors," Chem. Commun., (4), 441 (2005).

[1]work in collaboration with Gunnar Rueckner