Self-propulsion at the Nano-scale by Exponential Kicks

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Downsizing of active matter to the nano-scale is one of the main challenges in the field [1]. A class of propulsion mechanisms at the micro-scale relies on gradients (self-phoresis). In particular, local heating by laser of Janus colloids has been demonstrated to produce self-thermophoresis [2].

With a proof-of-concept model (fullerene of diameter ≈ 1 nm, with an idealized dipole attached to one end), we showed that asymmetric energy transfer is also a viable mechanism for propulsion at molecular scales. In water, this system presented self-thermophoresis as a result of periodic dipole inversions [3].

Prompted by the success of this model, an all-atom study of the vibrational dynamics of nitromethane has been carried out [4] based on a robust *ab-initio* classical force field [5]. This is the smallest molecule that, due to its amphiphilic character, one can expect asymmetric energy transfer to the surrounding solvent. We have found that the relaxation of high energy vibrational excitations indeed displays a high degree of spatial asymmetry.

Following this study, simulations of periodic excitations resulted in spontaneous propulsion, in the form of short time kicks, well represented by exponentially decaying center of mass velocity pulses [6]. The intensity and characteristics of these kicks are largely dependent on the excited mode, which our all-atom approach allows us to study with precision. To our knowledge, this is the first instance of molecular scale autonomous propulsion based on local anisotropy generated by the molecule (after excitation by external radiation).

While propulsion from exponential kicks has been found in a multitude of active systems, from schools of fish [7] to Janus colloids [8], our work presents the first instance of such phenomenon at the nano-scale. We have used analytic models to

obtain analytic expressions for the diffusion of such systems [9]. We found that propulsion can be greatly enhanced by time dependence in comparison to constant velocity propulsion, common in active matter studies. Such enhancements could prove key to overcoming the diffusional rotational damping prominent at small scales.

References

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