

## Self-Thermophoresis at the Nanoscale Using Light Induced Solvation Dynamics

Carles Calero<sup>C, S</sup>

*Department of Condensed Matter Physics, Universitat de Barcelona, Barcelona, Catalunya, Spain*  
*carles.calero@ub.edu*

Rosend Rey

*Department of Physics, Universitat Politecnica de Catalunya, Barcelona, Catalunya, Spain*

Edwin L. Sibert III

*bDepartment of Chemistry and Theoretical Chemistry Institute, University of Wisconsin-Madison, Madison, Wisconsin, U.S.A.*

Downsizing microswimmers to the nanoscale, and using light as an externally controlled fuel, are two important goals within the field of active matter. Here we report on a theoretical calculation showing that enhanced diffusion may be achieved at the nanometer scale using well-tuned electromagnetic radiation, simultaneously avoiding optical trapping. We demonstrate using all-atom molecular dynamics simulations that solvation relaxation, the solvent dynamics induced after visible light electronic excitation of a fluorophore, can be used to propel nanoparticles immersed in polar solvents. We show that fullerenes functionalized with fluorophore molecules in liquid water exhibit substantial enhanced mobility under external excitation, with a propulsion speed proportional to the power dissipated into the system. We show that the propulsion mechanism is quantitatively consistent with a molecular scale instance of self-thermophoresis. Strategies to direct the motion of functionalized fullerenes in a given direction using confined environments are also discussed.