Universität Basel

Research Project

Molecular Nanorovers: A roadmap to molecular superlubricity

Third-party funded project

Project title Molecular Nanorovers: A roadmap to molecular superlubricity
Principal Investigator(s) Vilhena Albuquerque D'Orey, José Guilherme ;
Co-Investigator(s) Meyer, Ernst ;
Organisation / Research unit
Departement Physik / Nanomechanik (Meyer)
Department
Project start 01.03.2020
Probable end 28.02.2021
Status Completed

Understanding and choreographing the dance of molecules is a matter of utmost complexity as not only requires a detailed knowledge of their intricate internal dynamics but also how the latter affects and is influenced by its surroundings. Fueled by the practical interest of controlling molecular motion/diffusion in organic synthesis, catalysis, . . . , throughout history we witnessed ever ingenious ways to control/activate the motion of molecules: from the plain old heating and stirring, up to microwave and laser guided molecular streams[1]. Yet, a seemingly control of molecular motion at solid interfaces has thus far remained elusive. The challenge stems from understanding how an external stimuli (e.g. light, electrical or chemical energy) can be harnessed to induce structural modifications or alter molecule-surface interactions in such way that generates motion. Such understanding would benefit not only the surface chemistry at large (e.g. on-surface synthesis[2] and catalysis[3]) but also the growing community of nanoscale synthetic molecular machines[4,5] since most their biomolecular counterparts operate at interfaces[6]. The difficulty to direct the motion of molecules over surfaces is perhaps best realized considering that in the 1st nanocar/molecular race[7] only two out of 7 world class research groups were able to meet the challenge. This consisted in propelling a molecule (each team could bring its "best contender") along 100nm in less than 30h!! The sole molecules crossing the finish line required a large amount of time (considering the distance), were very small molecules and used extremely energy inefficient propelling mechanisms.

In this project we propose a novel strategy consisting in a bottom-up chemical design of molecules that explore recent advances in superlubricity and physical chemistry allowing to decrease the energy dissipated during the motion by one order of magnitude. Whats more, this will enable to remotely/autonomously propel the molecules

along well
defined directions using simply an external uniform electric field. To meet this ambitious goal we resort to a synergetic
approach combining state of the art 5K Ultra High Vacuum Scanning Probe Microscopy (UHV-SPM) experiments with
all atom molecular dynamics simulation (MD) with parameters derived a priory from Quantum Mechanical (QM)
calculations. This Spark project will enable the transition of molecular propelling from pulses to fields (STM pulses to
uniform electric fields).

Financed by
Swiss National Science Foundation (SNSF)

Add publication

Add documents

Specify cooperation partners