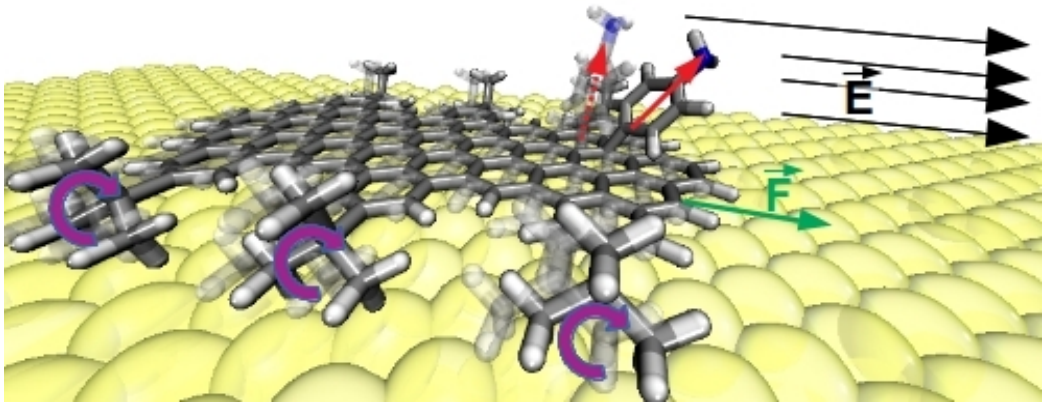
Nanomachines & Molecular Nanorovers

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 so 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 all atom molecular dynamics simulations feed with inter-atomic potentials (i.e. force fields) sourced from quantum mechanical calculations so to describe molecular vibrations with the ultimate resolution. This project will spark the transition of molecular propelling from local pulses to remote fields.



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References:
[1] Sugiyama, et al. **Accounts of Chemical Research**, 45(11), 1946–1954 (2012). **[2]** Niko Pavliček, et al. **Nature Nanotechnology**, 12(4), 308–311 (2017). **[3]** Cheng Hao Wu, et al. **Nature Catalysis**, 2(1), 78–85 (2019). **[4]** D. Sluysmans et al. **Proceedings of the National Academy of Sciences**, 115(38), 9359–9361. (2018) **[5]** Tibor Kudernac, et al. **Nature**, 479(7372), 208–211 (2011). **[6]** D. Lensen et al. **Soft Matter**, 8(35), 9053–9063 (2012). **[7]** G. Rapenne et al. **Nature Reviews Materials**, 2, 1–3 (2017).