

# Propulsion from energy bursts for nitromethane in water

Arnau Jurado Romero<sup>1</sup>, Carles Calero Borrallo<sup>2</sup>, and Rossend Rey Oriol<sup>1</sup>

<sup>1</sup>Universitat Politècnica de Catalunya, Jordi Girona, 1-3. B5, 08034 Barcelona

<sup>2</sup>Universitat de Barcelona, Martí i Franquès, 1, 11, 08028 Barcelona

Energy dissipation is of interest for the accurate generation and control of movement in micro and nano-particles. Studying molecular relaxation after a vibrational excitation has potential applications in multiple fields.

We consider the nitromethane molecule, whose energy relaxation after vibrational excitation has already been studied in argon gas [1, 2].

Prompted by the amphiphilic nature of nitromethane we study its relaxation in liquid water. We perform high energy excitations (200 kJ/mol) of individual modes and study energy relaxation via all-atom molecular dynamics simulations.

Our results show that, as expected, some normal modes relax considerably faster than others. These faster modes have associated motions related to the nitro group, which is to be expected due to the hydrophilic nature of the functional group.

To get more insight into the relaxation mechanisms we also studied the work performed by the nitromethane molecule on the surrounding water molecules [3]. Our main finding is that energy relaxation is remarkably asymmetric, favoring the nitro side (30% more work is performed to the nitro side).

To our knowledge this is the smallest molecule for which a marked asymmetry has been found, irrespective of the excited mode.

A combination of fast relaxation, asymmetry and translational work result in a short time impulse for select mode excitations. Repeated excitations result in enhanced diffusion.

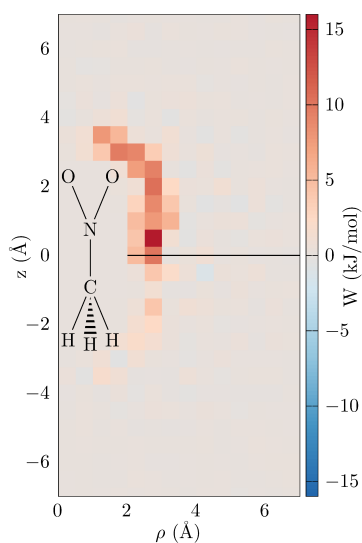


Fig. 1. Spatial distribution of the net work exerted by a nitromethane molecule on its liquid water environment once vibrational relaxation is complete, averaged over a set of microcanonically distributed excitations of 200 kJ/mol.

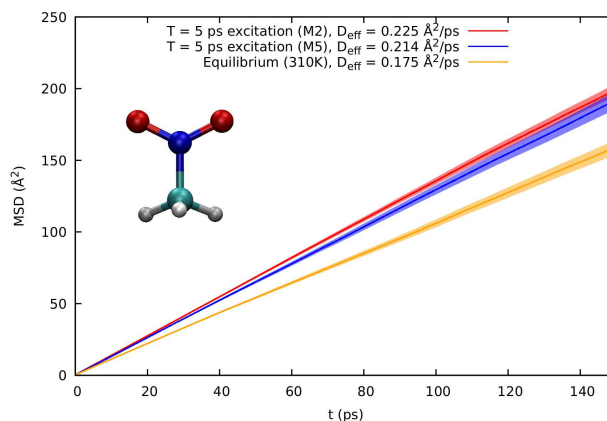


Fig. 2. Mean square displacement for repeated excitations of select normal modes of nitromethane and for equilibrium.

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[4] Calero, C., Sibert E. L. III, and Rey, R. *Nanoscale* **12** 7557 (2020)

[5] Jurado Romero, A., Calero, C., Sibert, E. L. III, and Rey, R., *J. Chem. Phys.* **158**, 194501 (2023).