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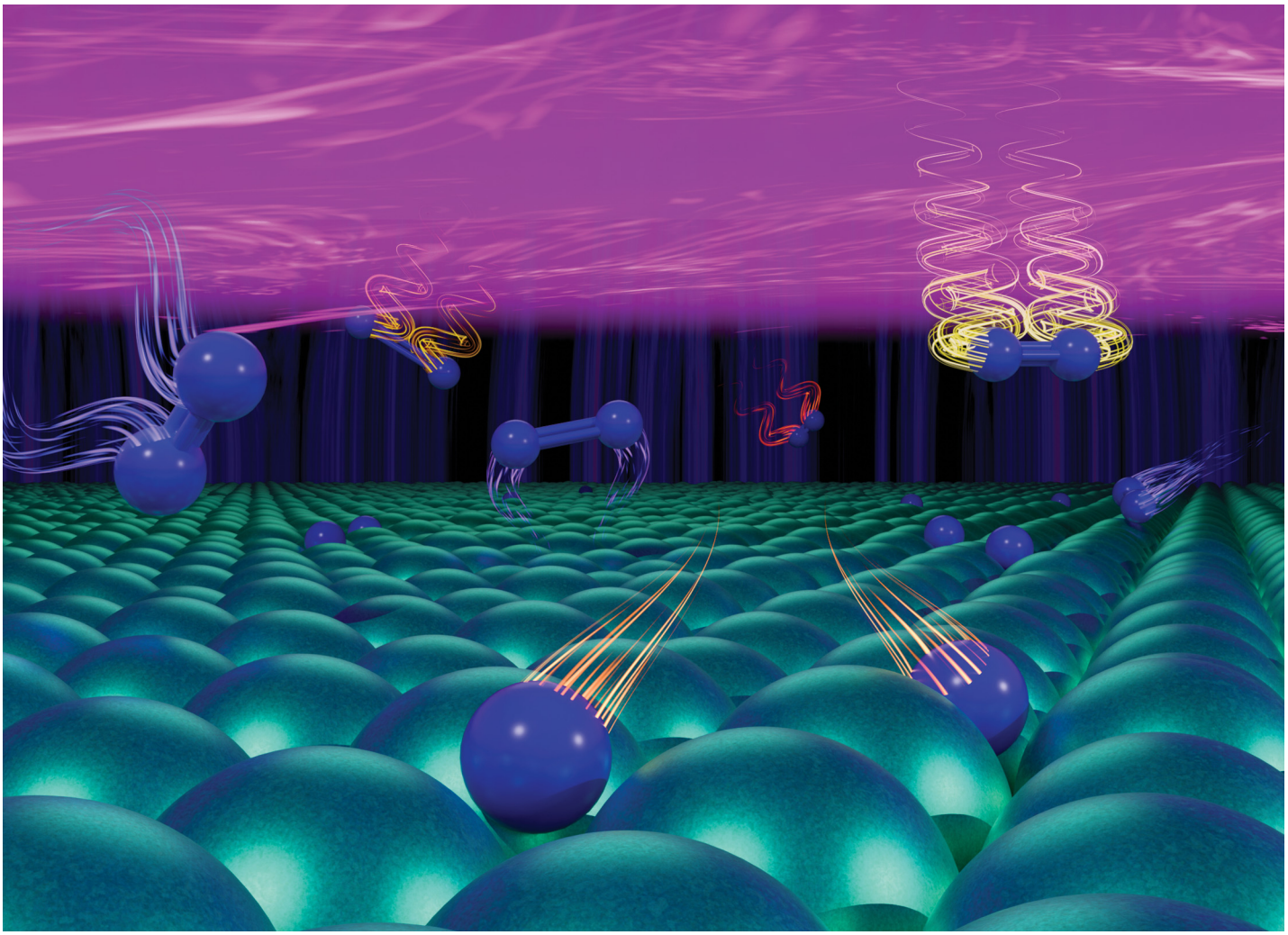

Showcasing research from the group of Dr Jörg Meyer, Theoretical Chemistry, Leiden Institute of Chemistry, Leiden University, The Netherlands.

Vibrational excitation in plasma catalysis: how important are dynamical effects?

Vibrationally excited N_2 molecules have been suggested to boost the efficiency of heterogeneously catalysed ammonia synthesis, where N_2 dissociation on a metal surface is the rate-determining step. To quantify the enhancement of the dissociation rate coefficient relative to N_2 molecules in the vibrational ground state, we have performed molecular dynamics simulations in the quasi-classical framework on accurate high-dimensional potential energy surface obtained from density functional theory calculations. The enhancement is significantly more pronounced than found previously based on the so-called Fridman–Macheret α model, which has important implications for both thermal and plasma-enabled catalysis.

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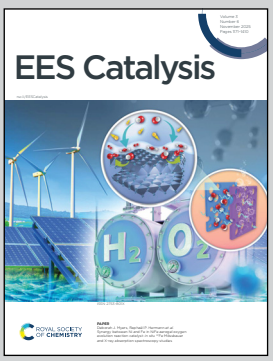

See Floris van den Bosch *et al.*, *EES Catal.*, 2025, **3**, 1257.

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