Stochastic Simulations of Energy Exchange at Surfaces

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In this contribution, we explore the dissipative dynamics of a multidimensional system in contact with a Markovian bath in the weak and strong coupling regimes. In this endeavour, we use the recently developed stochastic Multi-Configuration Time-Dependent Hartree approach within the Monte Carlo wave packet formalism [J.\,Chem.\,Phys.\,156, 094109 (2022)]. The method proved to yield thermalized ensembles of wave packets when intramolecular coupling is weak.

A model two-dimensional Hamiltonian parameterized to represent an adsorbate-surface system is investigated to disentangle the effects of intramolecular potential coupling, of strong mode mixing observed in Fermi resonances, and of anharmonicity. Further, we simulate state-to-state scattering dynamics of NO on Au(111) to reveal important orientational effects due to vibrationally quantized relaxation.