Relaxation and quantum diffusion of CO on metallic surfaces

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We investigate the excitation and relaxation dynamics of diatomic molecules adsorbed on metallic surfaces using a model Hamiltonian which resembles that of CO on Cu(100) [1]. The model accounts both for diffusion and desorption of the molecular adsorbate. The dissipative dynamics is simulated using the reduced density matrix in its Lindblad form. An explicit expression for the evaluation of position-dependent transition rates in an optimized DVR is introduced. A wide range of coupling strengths between the different degrees of freedom is considered. The influence of the dimensionality on the energy redistribution among the vibrational and translational modes is explored.

References:
[1] Tremblay J. C., Füchsel, G., Saalfrank P., Physical Review B, 2012, 86, 045438