Electronic Supplementary Information:

Scattering of NO(ν=3) from Au(111): a stochastic dissipative quantum dynamical perspective

Tobias Serwatka,* Gernot Füchsel* and Jean Christophe Tremblay†

---

*Institut für Chemie und Biochemie, Freie Universität Berlin, D-14195, Germany

†Laboratoire de Physique et Chimie Thoriques CNRS-Universit de Lorraine, UMR7019, ICPM, 1 Bd Arago, 57070 Metz, France.

1 Convergence test

The following figures depict the vibrational and rotational distributions of the scattered molecules for initial translational energies ranging from 0.2 eV to 0.6 eV. The distributions are depicted for all high-symmetry sites (top, hcp, fcc).
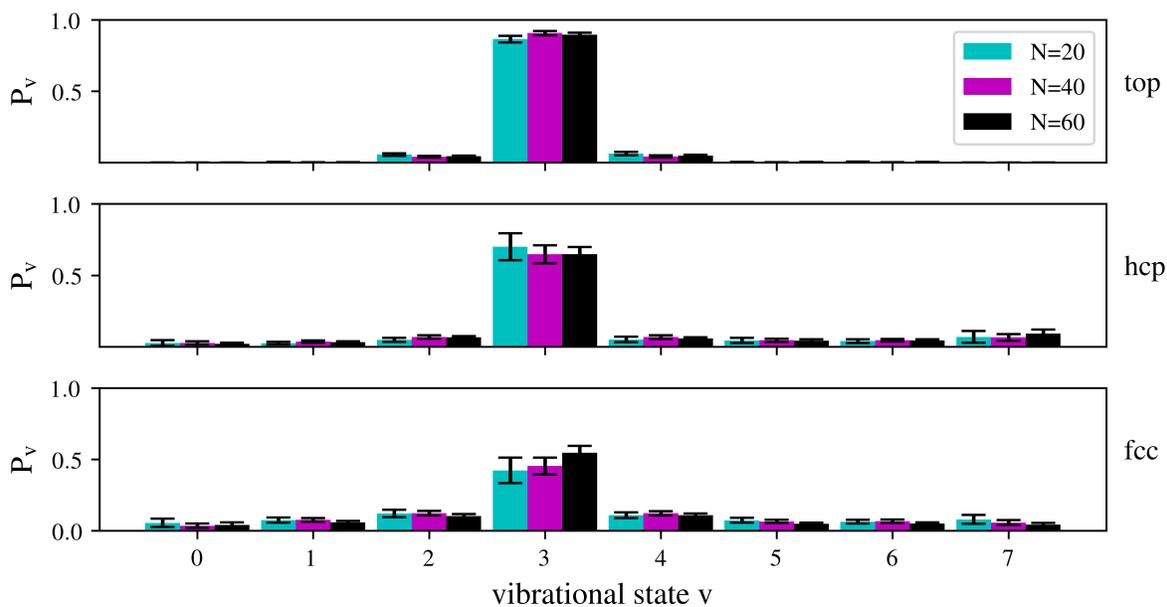
Vibrational distribution

Figure S1: Vibrational distribution of NO molecules scattered at normal incidence with an initial translational energy of 0.2 eV, averaged over 20 (cyan), 40 (magenta) and 60 (black) realizations. The black bars indicate the statistical error on the averaged values.
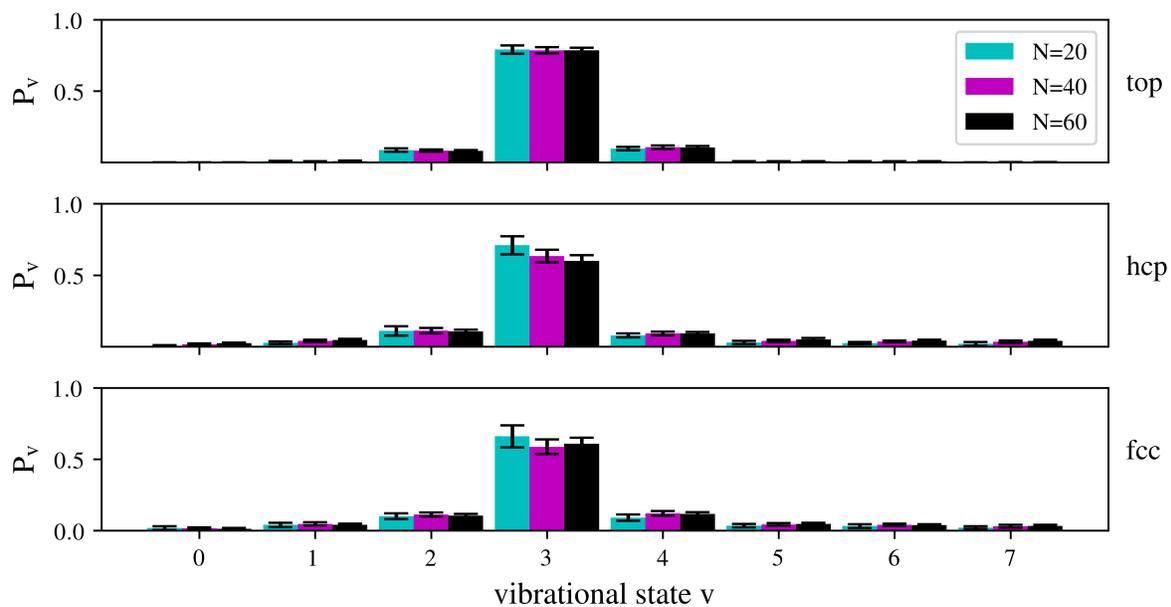
Figure S2: Vibrational distribution of NO molecules scattered at normal incidence with an initial translational energy of $0.6\,\mathrm{eV}$, averaged over 20 (cyan), 40 (magenta) and 60 (black) realizations. The black bars indicate the statistical error on the averaged values.
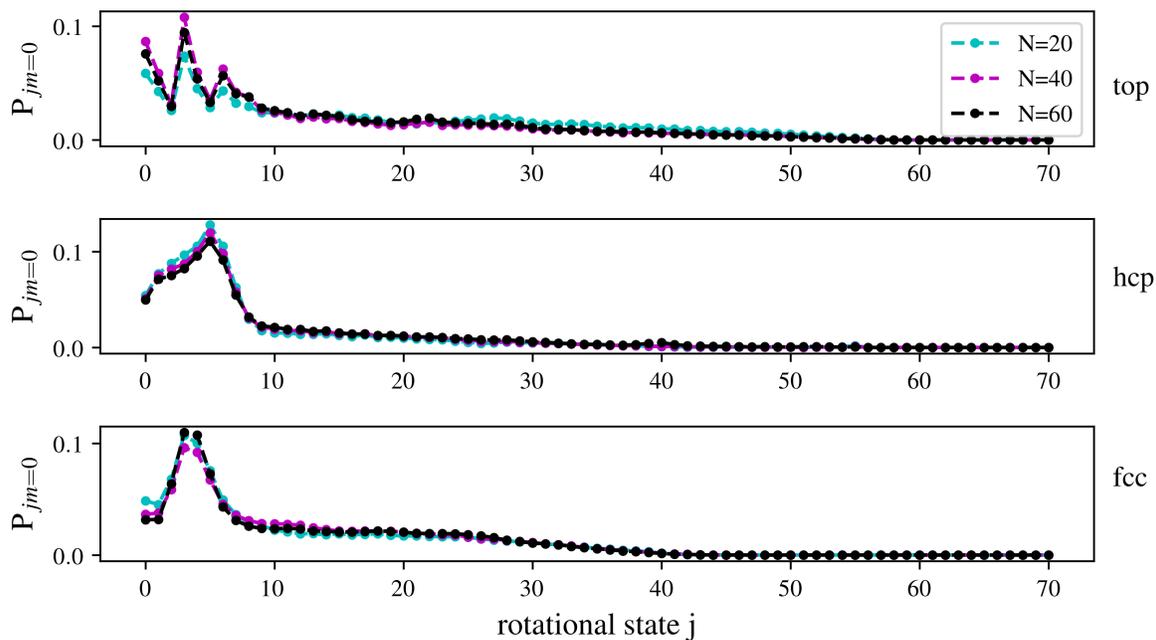
Rotational distribution

Figure S3: Rotational distribution of NO molecules scattered at normal incidence with an initial translational energy of $0.2\,\mathrm{eV}$, averaged over 20 (cyan), 40 (magenta) and 60 (black) realizations. The black bars indicate the statistical error on the averaged values.

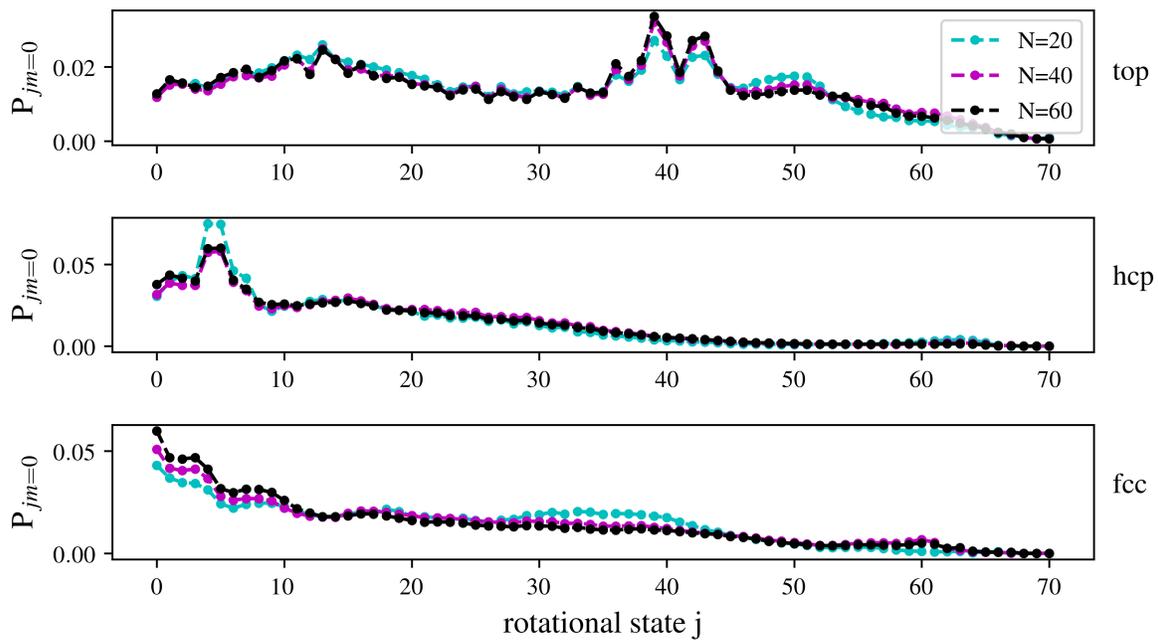Figure S4: Rotational distribution of NO molecules scattered at normal incidence with an initial translational energy of $0.6\,\mathrm{eV}$, averaged over 20 (cyan), 40 (magenta) and 60 (black) realizations. The black bars indicate the statistical error on the averaged values.

2   Time-dependent vibrational state population

The following figures show the time-dependent population of internal vibrational states of NO for scattering from Au(111) at the top and the fcc sites with an initial translational energy of 0.2 eV. The internal vibrational states are defined as the eigenstates of the vibrational Hamiltonian in the gas phase for $j = 0$. The results are show for purely determinstic simulations, i.e., without dissipation, to reveal the topological nature of the population transfer process during the impact.
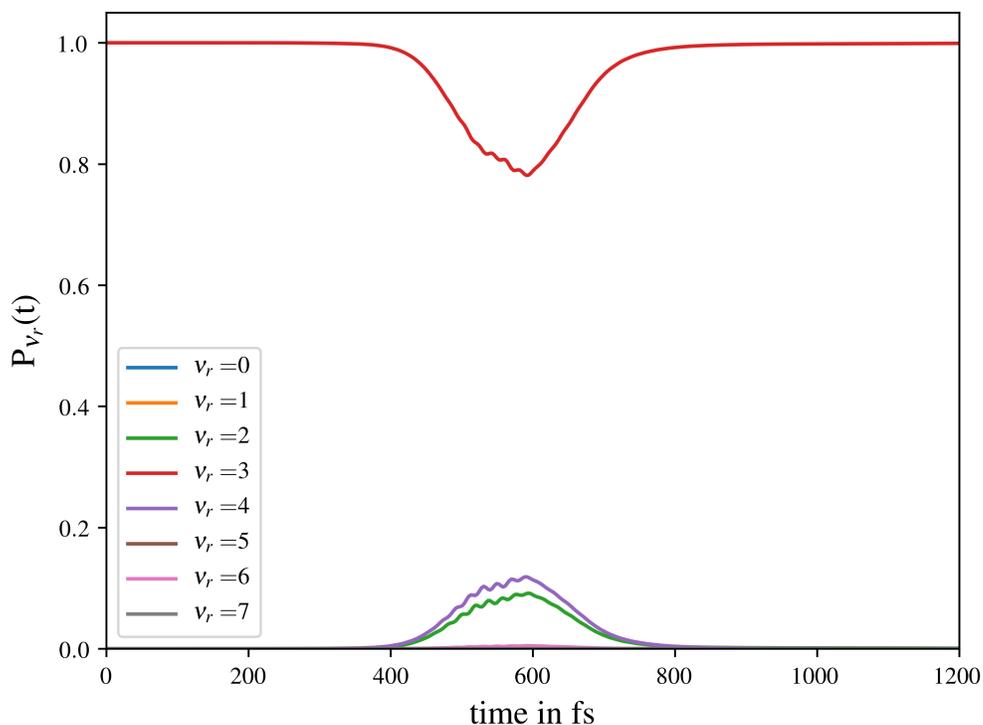

Figure S5: Time-dependent population of the internal vibrational states of NO for scattering from Au(111) at the top site with an initial translational energy of 0.2 eV.
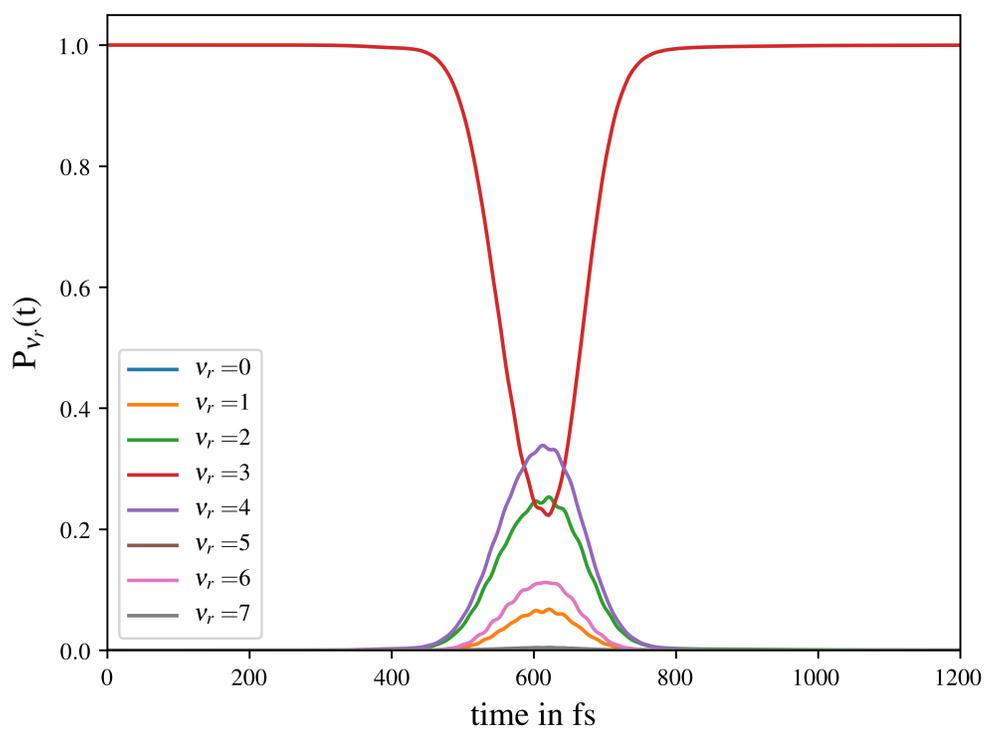
Figure S6: Time-dependent population of the internal vibrational states of NO for scattering from Au(111) at the fcc site with an initial translational energy of $0.2\,\mathrm{eV}$.