# Energy dissipation channels in the reflection and adsorption of nitrogen on Ag(111)

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In this work, we investigate the scattering of N atoms on Ag(111) surfaces. Our calculations rely on an accurate potential energy surface based on density functional theory (DFT) calculations. Interpolation of the DFT data is performed using the corrugation reducing procedure [1]. Dynamics is studied using a Monte Carlo sampling and classical trajectories. In particular, this study focuses on the role played by electron and phonon excitations in the reflection and adsorption processes. Energy dissipation to the metallic surface through phonons is taken into account with the Generalized Langevin Oscillator model. Electron-hole pairs excitations are also included using a local friction coefficient [2]. Regarding the reflection process, our theoretical results are in reasonable agreement with recent experimental data [3]. We show that phonon excitation is responsible for the energy loss observed experimentally whereas electron-hole pair excitations represent a minor contribution. Nevertheless, a detailed study of the adsorption mechanism points out that the combination of electronic and phonon excitations is necessary to properly describe the full dynamics of this elementary reactive process.

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