Nitrogen atoms and molecules landing, reacting, and rebounding at metal surfaces

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Advances in gas-surface dynamics are largely triggered by the quest for systems and conditions under which reactivity can be controled, enhanced or inhibited. Nitrogen on metal surfaces is a common subject of studies in this field. The closed shell nature of molecular N_2, as well as its high binding energy, makes the molecule quite inert. In contrast, atomic N is generally reactive, recombines easily with other atoms, and strongly adsorbs at surfaces. This dichotomy turns the Nitrogen dynamics at surfaces into a rich and intriguing problem.

Here we review recent theoretical work on elementary reactive processes taking place when Nitrogen atoms and molecules interact with clean and decorated metal surfaces [1-4]. The theoretical framework relies on ab-initio built potential energy surfaces and full-dimensional classical dynamics. Energy exchange with the surface is included through the excitation of electron-hole pairs and phonons. We actually evaluate the role of these two energy dissipation channels in the scattering and adsorption of N_2 on W(110) and N on Ag(111) [1-2]. We show that, in atomic N adsorption, phonons are responsible for determining the adsorption probability but electronic excitations are relevant at a later stage to fix the atoms to the adsorption positions. In the case of N atoms incident on N-covered Ag(111), we show that the Eley-Rideal recombination process between gas-phase N atoms and N adsorbates is a highly efficient mechanism for N_2 formation [3]. Finally, we show that strain can be a useful tool to promote reactivity: N_2 molecules adsorb and dissociate with higher rates at the strained Fe/W(110) surface than at the Fe(110) surface [4]. We conclude that relatively small variations in interaction energies can lead to drastic changes in the dynamics and thus to modifications in the final output of the scattering process.

References

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