

## Séminaire de Chimie Théorique

Salle Réunion, 4eme Ouest, bat. A12

Vendredi 30 Juin à 11:00

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### **Hydrogen atom scattering from metal surfaces: Molecular dynamics with electronic friction on a full-dimensional Potential Energy Surface.**

Experiments probing inelastic scattering of H atoms from a metal surface show that the translational energy losses are dominantly due to electronic excitations of the surface. The molecular dynamics simulations on the full-dimensional potential energy surface with accounting for the nonadiabatic effects on the level of the electronic friction give good agreement with those experimental results for various incidence conditions, thus, providing the insight into the energy transfer processes during the scattering.).

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