Modelling energy dissipation for molecules at surfaces

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In the dawning age of sustainability, energy harvesting and dissipation at interfaces play a crucial role for processes that feed and fuel our modern societies. At the atomic scale, the vibrational lifetime of small molecular adsorbates can provide detailed information about the molecular dynamics of energy exchange with the surface [1]. The most obvious dissipation channel is given by vibrations of the surface atoms (phonons). However, while elucidating the energy transfer dynamics for vibrationally excited CO adsorbed on a NaCl(100) surface, we have recently identified the important contribution of another dissipation mechanism [2]. In case of metal surfaces the excitation of electron-hole pairs is commonly believed to be the most dominant dissipation channel [3]. This challenges computational modelling to go beyond the ubiquitous Born-Oppenheimer approximation. Numerically appealing electronic friction [3] schemes have attracted a lot of interest in order to include the effects of electron-hole pair excitations in (classical) molecular dynamics. I will compare different ways to calculate the electronic friction coefficients and discuss the effects on vibrational damping of CO adsorbed on Cu(100) and on Pt(111) surfaces [4,5]. Finally, I will conclude with implications for reactive scattering of H2 from Cu(111) [6] and N2 from Ru(0001) [7].

**References**

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