

fs-laser-driven dynamics of CO on Ru(0001)

a computational study using electronic friction (MDEF) and
the generalized Langevin oscillator (GLO)

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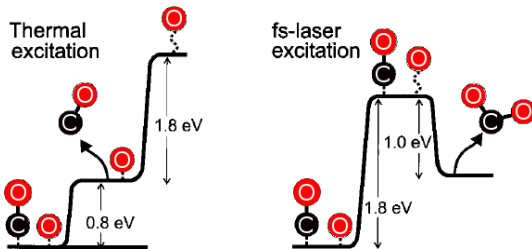
- 1 Introduction
 - Motivation

- 2 models and methods

General motivation

Why investigate fs-laser-driven surface dynamics?

- gain fundamental understanding of adsorbate bonding
⇒ additional tool besides scattering experiments
- possible direct application in catalysis: “femtochemistry”
⇒ new reaction pathways opened up by fs-lasers



CO/O-coadsorbate @ Ru(0001)

M. Bonn *et al.*, SCIENCE 1999

Specific motivation for the CO/Ru-System

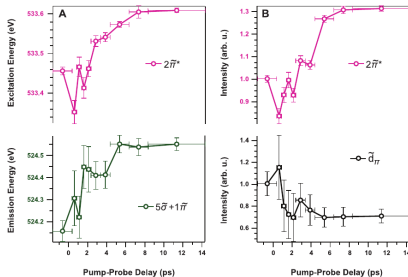
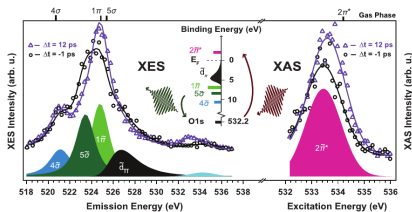
CO/Ru system important for catalysis

e. g. Fischer-Tropsch synthesis

Experimentally well studied system

- especially regarding fs-laser irradiation e.g. Bonn, SCIENCE 1999 and Funk J. CHEM. PHYS 2000 (Ertl group - chemistry Nobel prize 2007).
- recently, time resolved x-ray spectra (XAS and XES)
⇒ “movie” of changes in orbital DOS

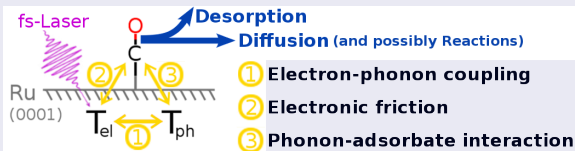
Details of the experiment



What happens after fs-laser excitation of the metal?

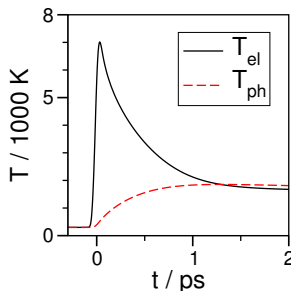
Coupling between three different kinds of degrees of freedom:

- electron gas (T_{el})
- lattice vibrations (T_{ph})
- adsorbate movement (T_{ads})



Two-Temperature Model

$$C_{\text{el}} \frac{\partial T_{\text{el}}}{\partial t} = \frac{\partial}{\partial z} \kappa \frac{\partial}{\partial z} T_{\text{el}} - g(T_{\text{el}} - T_{\text{ph}}) + S(z, t),$$
$$C_{\text{ph}} \frac{\partial T_{\text{ph}}}{\partial t} = g(T_{\text{el}} - T_{\text{ph}}).$$



Laser-Driven Diffusion

