

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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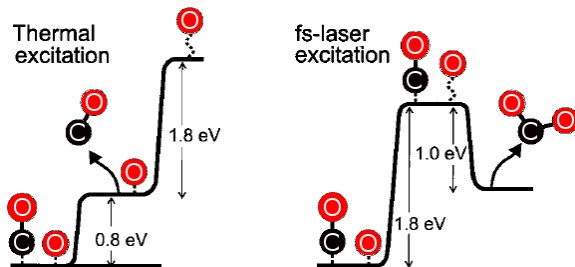
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- 1 Introduction
 - Motivation

General motivation

Why investigate fs-laser-driven surface dynamics?

- gain fundamental understanding of adsorbate bonding
- 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

Recent Experiments partly contradict theory

- Ultrafast time-resolved X-Ray-sepctroscopy hints to physisorbed precursor state
- Recent full 6D PES does not feature physisorption well

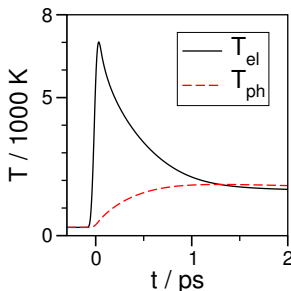
Open questions for theory

- Do dynamics reproduce other observables correctly? (e. g. desorption yield)
- Can the X-Ray-spectra also be explained without physisorption?

Details of the experiment

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

