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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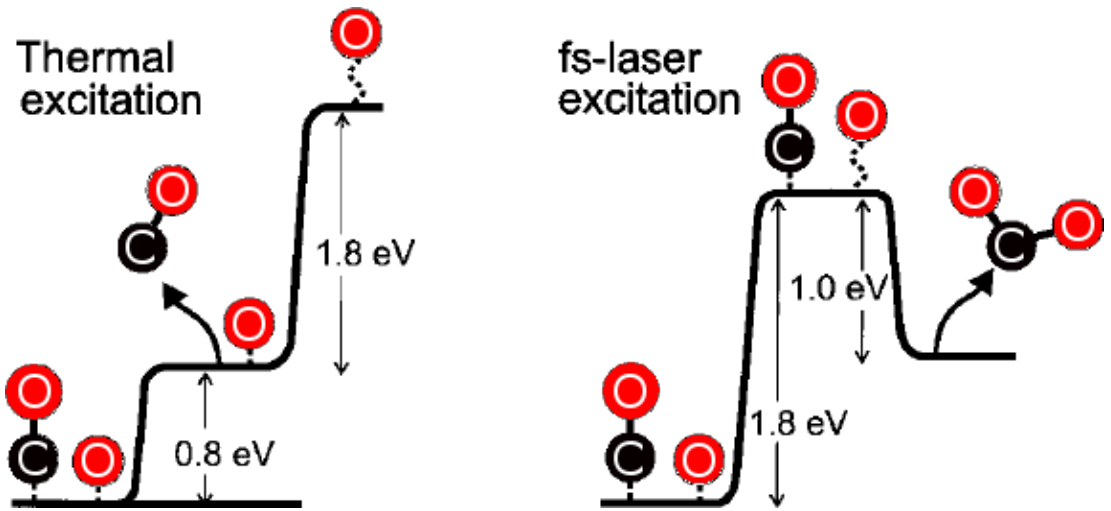
General motivation

Why investigate fs-laser-driven surface dynamics?

- gain fundamental understanding of adsorbate bonding
  $\Rightarrow$ additional tool besides scattering experiments
- possible direct application in catalysis: “femtochemistry”
  $\Rightarrow$ 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

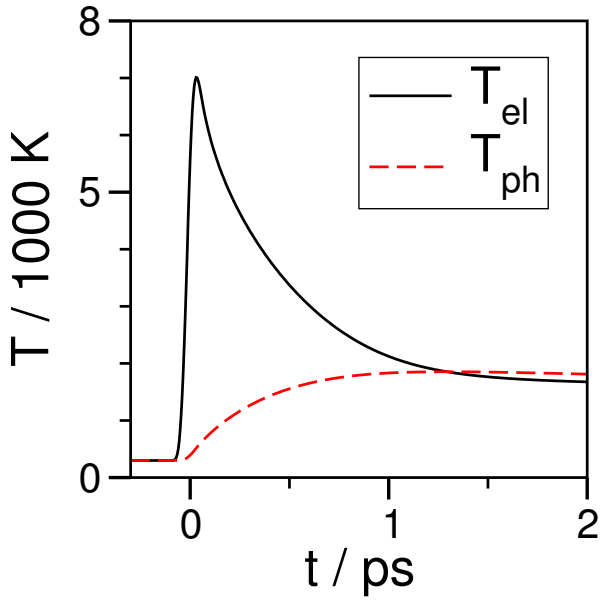
- Do dynamics reproduce other observables correctly? (e. g. desorption yield)
- Can the X-Ray-spectra also be explained without physisorption?

Details of the experiment

Two-Temperature Model

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

$$C_{\mathrm{ph}} \frac{\partial T_{\mathrm{ph}}}{\partial t} = g(T_{\mathrm{el}} - T_{\mathrm{ph}}).$$



Laser-Driven Diffusion