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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Gliederung

General motivation

Why investigate laser-driven dynamics on surfaces?

- possible new reaction pathways in heterogenous catalysis
- laser induced desorption, diffusion and reactions
- for fundamental understanding of adsorbate bonding and catalysis

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

Laser-Driven Diffusion