

FEMTOSECOND-LASER INDUCED DYNAMICS OF CO ON Ru(0001): NEW INSIGHTS FROM A
HOT-ELECTRON, ELECTRONIC FRICTION MODEL INCLUDING SURFACE MOTION

Robert Scholz^{1,2}, Gereon Floß¹, Peter Saalfank¹, Gernot Fuchsels³, Ivor Lončarić⁴, and J. I. Juaristi^{4,5,6}

¹Institut für Chemie, Universität Potsdam, Karl-Liebknecht-Str. 24-25, D-14476 Potsdam, Germany

²Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany

³Universiteit Leiden, Gorlaeus Laboratories, Einsteinweg 55, 2333 Leiden, The Netherlands

⁴Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), Paseo Manuel de Lardizabal 5, 20018 Donostia-San Sebastián, Spain

⁵Departamento de Física de Materiales, Facultad de Químicas, Universidad del País Vasco (UPV/EHU), Apartado 1072, 20080 San Sebastián, Spain

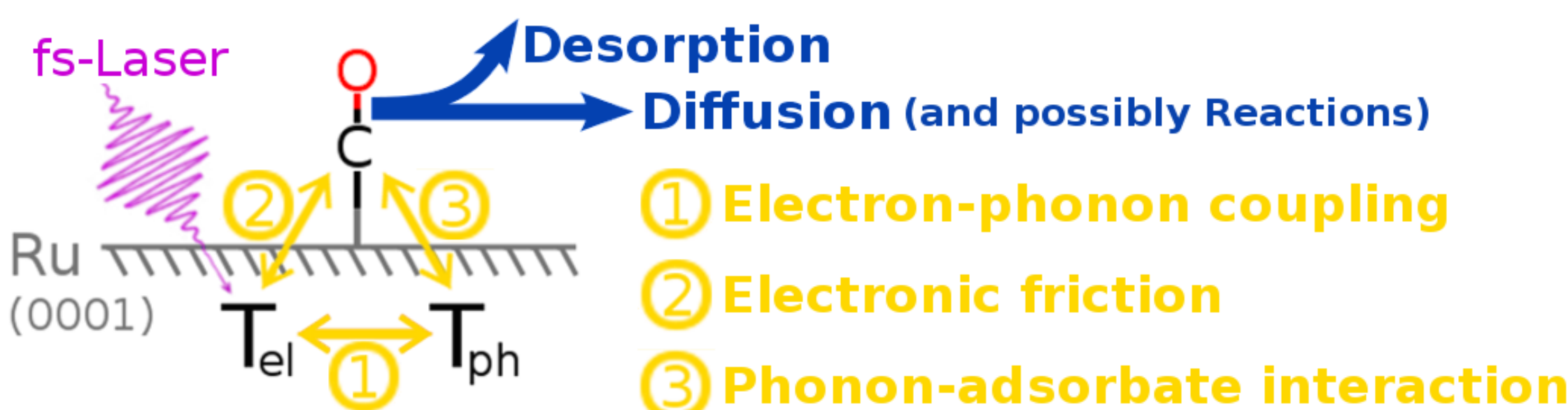
⁶Donostia International Physics Center DIPC, P. Manuel de Lardizabal 4, 20018 San Sebastián, Spain

Introduction

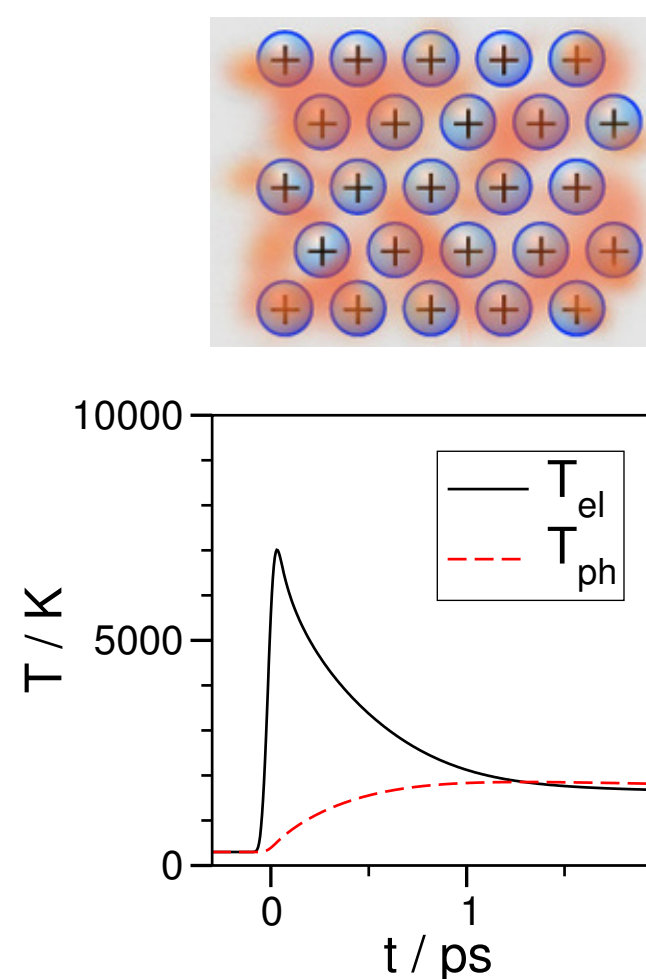
Motivation

- research on small molecules adsorbed to metals is important for:
 - catalytic applications
 - fundamental understanding of bonding
- femtosecond(fs)-lasers are a valuable tool for such research as they
 - allow for investigations on small timescales
 - open up new processes compared to heating (femtophotocchemistry)
 - may enable specific control over catalytic reactions (photocatalysis)

How does fs-laser-irradiation affect metal surfaces?



- metals: ion lattice plus quasi-free electron gas
- visible light is absorbed only by the electrons
- electrons transfer part of energy to ion lattice, via **① electron-phonon coupling** (phonons = lattice vibrations)
 - electrons couple to phonons as their fast movement causes “shockwaves” in ion lattice
 - equilibration process completes after ~ 1 ps
- Thus, with fs-lasers, two temperatures emerge:
 - T_{el} - electron temperature
 - T_{ph} - phonon temperature
- time evolution can be simulated with a Two-T



Models and Methods

Potential Energy Surface

Electronic Friction: LDFA and Langevin Dynamics

Inclusion of Phonons: GLO-model

References

- [1] S. I. Anisimov, B. L. Kapeliovich, and T. L. Perel'man, *Sov. Phys.-JETP* **39**, 375 (1974)

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