JOHANNES KEPLER
UNIVERSITÄT LINZ

# Sonderkolloquium

**Fachbereiche Chemie und Physik**

Im Rahmen eines Sonderkolloquiums der Fachbereiche

Chemie und Physik spricht

**Prof. Dr. Reinhard J. Maurer**

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über

## Hot electrons in surface chemistry: From molecular scattering to plasmonic catalysis

Nonadiabatic effects that arise from the concerted motion of electrons and atoms at comparable energy and time scales are omnipresent in thermal and light-driven chemistry at metal surfaces. Short-lived excited (hot) electrons can measurably affect molecule-metal reactions by introducing energy dissipation, dynamical steering effects, and by contributing to state-dependent reaction probabilities. [1] Furthermore, hot electrons, created by plasmonic excitation upon light exposure, can selectively activate chemical reactions at metal catalyst surfaces. I will present our recent efforts to establish molecular dynamics methods able to capture nonadiabatic and quantum effects at metal catalyst surfaces. We employ a range of methods to capture hot electron effects such as molecular dynamics with electronic friction and surface hopping dynamics. By combining linear response electronic structure calculations [2] with high-dimensional machine-learning representations, [3] we are able to perform ensemble-averaged nonadiabatic dynamics at surfaces. I will showcase this for the vibrational state-to-state scattering of NO on Au(111), [4] where we can identify the regimes in which electronic friction is valid. I will also provide a detailed analysis of the limitations of the existing approach and our ongoing efforts to include quantum tunnelling effects, memory effects, and explicit excited-state effects to capture the dynamics of light-driven hot-electron chemistry.

[1] Bartels et al, *Chem. Sci.* **2**, 1647−1655 (2011)

[2] R. J. Maurer, M. Askerka, V. S. Batista, J. C. Tully, *Phys. Rev. B* **94**, 115432 (2016)

[3] Y. Zhang, R. J. Maurer, B. Jiang, *J. Phys. Chem. C* **124**, 186-195 (2020)

[4] C. L. Box, Y. Zhang, R. Yin, B. Jiang, R. J. Mauer, *JACS Au* 1, 164–173 (2021)

Datum: Do, 2.6.2022 Zeit: 14:00 via ZOOM

https://jku.zoom.us/j/97423054839?pwd=MHRuMEJNdFl4a0tOcXBsNW40OVR6UT09

Meeting-ID: 974 2305 4839 Passwort: 032600