

## SYED 1: Symposium Electron-driven processes

Time: Thursday 9:30–12:15

Location: HSZ 01

**Invited Talk**

SYED 1.1 Thu 9:30 HSZ 01

**Ultrafast electron dynamics at laser-irradiated surfaces** — ●BAERBEL RETHFELD — Department of Physics and Research Center OPTIMAS, Technische Universität Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany

When a femtosecond laser pulse of moderate intensity irradiates a solid surface, the energy is mainly absorbed by the electrons within the crystal. We calculate numerically the transient distribution function of laser-excited electrons with help of full Boltzmann collision integrals. Based on their density of states, we can trace different materials' response to an ultrafast stimulus of photonic excitation, as well as the interplay of electron-electron and electron-phonon interaction. Our results show that the initial characteristic signatures of the energy absorption are thermalized on a timescale of a few femtoseconds up to tens of femtoseconds. However, the cooling of the heated electron system by the cold phonons induces a further nonequilibrium, persisting on picosecond timescales [1].

We present possible consequences of the electron-phonon interaction on the energy distribution of hot electrons in dependence on material properties like band gap or particular features of the density of states.

[1] S.T. Weber and B. Rethfeld, Phys. Rev. B **99**, 174314 (2019)

**Invited Talk**

SYED 1.2 Thu 10:00 HSZ 01

**Unraveling Momentum-Dependent Electron-Phonon Coupling and its Role in the Origin of Charge Density Wave Phases** — ●BRADLEY SIWICK<sup>1,2</sup>, MARTIN OTTO<sup>1</sup>, JAN-HENDRIK POHLS<sup>1</sup>, LAURENT RENE DE COTRET<sup>1</sup>, and MARK SUTTON<sup>1</sup> — <sup>1</sup>McGill University, Department of Physics, Center for the Physics of Materials, Montreal, Canada — <sup>2</sup>McGill University, Department of Chemistry, Montreal, Canada

The nature of the couplings within and between lattice and charge degrees of freedom is central to condensed matter and materials physics. These interactions are essential to phenomena as diverse as superconductivity, charge density waves and carrier mobility in semiconductors and metals. Despite their fundamental role, detailed momentum-dependent information on the strength of electron-phonon coupling (EPC) and phonon-phonon coupling (PPC) across the entire Brillouin zone has proved elusive. This talk will describe a new technique, ultrafast electron diffuse scattering (UEDS), which provides such information. Specific applications of UEDS to 2D materials including graphite, TiSe<sub>2</sub> and TaSe<sub>2</sub> will be presented. The data demonstrate that UEDS patterns can separate the influence of the electronic susceptibility from the inelastic exchange of energy between the electron and phonon systems due to the technique's profound sensitivity to photoinduced changes to the phonon system. In TiSe<sub>2</sub>, this confirms key role of excitonic correlations to the phonon softening and CDW mechanism.

**Invited Talk**

SYED 1.3 Thu 10:30 HSZ 01

**Light MATTERS!!!** — ●HRVOJE PETEK<sup>1</sup>, ANDI LI<sup>1</sup>, ZEHUA WANG<sup>1</sup>, and MARCEL REUTZEL<sup>1,2</sup> — <sup>1</sup>Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania 15260, USA — <sup>2</sup>Present address: I. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany

Light interacting with solid-state matter under perturbative conditions excites primarily electric dipole transitions between k-vector dependent eigenstates of the periodic lattice potentials. A time-periodic light potential, however, can modify the electronic band structure of a solid through nonperturbative interactions entangling the light-matter interaction, and opening a route to tailor material properties with light at will. I will describe two examples: 1) It will happen at zero field strength when the complex dielectric response function  $\text{Re}[\epsilon(\omega)] \sim 0$  and  $\text{Im}[\epsilon(\omega)]$  is small. This happens for ionic solids above the longitudinal optical phonon frequency and for metals where the  $-\epsilon_\infty(\omega) \sim \epsilon_{\text{Drude}}(\omega)$ , or near the interband absorption threshold. This epsilon near-zero (ENZ) response coincides with the excitation of collective ion or electron responses, i.e., in case of metals, the bulk plasmon excitation. I will describe the ENZ response of single crystalline, low-index surfaces

of Ag, as measured by ultrafast multiphoton photoemission (mPP) spectroscopy. This bulk plasmonic response of Ag is fundamentally responsible for all plasmonic responses of silver, and yet the observed mPP spectra fundamentally contradict significant aspects that we expect from theory. 2) I will also report the high field response of Cu(111) surface where light is sufficiently strong to dress the electronic bands through Floquet engineering and Stark shift effects. The optical dressing opens the way to modify quasiparticles in solids at will, where, for example, electrons can be transformed into holes on subfemtosecond time scale. Our studies inform how light, electronic, and atomic degrees of freedom in solids can overcome their natural performance boundaries.

**15 min. break****Invited Talk**

SYED 1.4 Thu 11:15 HSZ 01

**Quantum localization and delocalization of charge carriers in molecular organic crystals** — ●JOCHEN BLUMBERGER — University College London, Gower Street, London, WC1E 6BT, UK

Charge carrier transport (CT) in organic semiconducting materials is at the heart of many exciting and revolutionising technologies. Yet, our fundamental understanding of CT in the active layers of these devices that could rationalise experimental observations and guide further advances in the field is still rather limited. Charge carriers in organic semiconductors (OSs) are often described by one of two extremes: by a travelling wave propagating through the material or by a particle hopping from one molecular fragment to the next. Here we show that neither of these simplified pictures applies. Solving the time-dependent electronic Schrödinger equation coupled to nuclear motion for eight different organic molecular crystals, we find that the excess charge carrier forms a polaron delocalized over 10-20 molecules in the most conductive crystals.[1] The polaron propagates through the material by diffusive jumps over several lattice spacings (nanometers) at a time during which it expands to about twice its size. Computed localization lengths and charge mobility are in excellent agreement with experimental estimates, where available, and exhibit strong positive correlation in agreement with the recently proposed transient localization theory.

[1] S. Giannini, A. Carof, M. Ellis, H. Yang, O. G. Zigos, S. Ghosh, and J. Blumberger, Nature Comm., vol. 10, p. 3843, 2019.

**Invited Talk**

SYED 1.5 Thu 11:45 HSZ 01

**Single-Atom Catalysis (SAC): How Structure Influences Reactivity** — ●GARETH PARKINSON — TU Wien, Vienna, Austria

The field of "single-atom" catalysis emerged as the ultimate limit of attempts to minimize the amount of precious metal used in heterogeneous catalysis. There are many reports of active catalysts for important heterogeneous, electrochemical and photocatalytic reactions, but it has become clear that metal adatoms behave very differently to supported nano-particles. This is because they form chemical bonds with the support and are often charged. Thus, SAC systems resemble coordination complexes used in homogeneous catalysis, and there is growing excitement that SAC could achieve similar levels of selectivity, and even "hetero-genize" problematic reactions currently performed in solution. Homogeneous catalysts are designed for purpose based on well-understood structure-function relationships, while in SAC, the complexity of real systems means that the structure of the active site is difficult to determine, never mind design. I will describe how we are using Fe<sub>3</sub>O<sub>4</sub>(001) as a precisely-defined model support to unravel fundamental mechanisms in SAC. First, I will describe systematic studies of CO adsorption across several metals (Cu, Ag, Au, Ni, Pt, Ir, Rh) and show that adsorbate-induced structural changes affect the stability of the catalyst and the desorption energy. Then I will describe how the local structure of Ir<sub>1</sub>/ and Rh<sub>1</sub>/Fe<sub>3</sub>O<sub>4</sub>(001) SACs change with preparation, and how CO adsorption stabilizes the system through square-planar and octahedral binding environments reminiscent of Ir<sub>1</sub> and Rh<sub>1</sub> based metalorganic complexes.