

O 80: Gerhard Ertl Young Investigator Award Competition

Time: Thursday 10:30–13:00

Location: TRE/PHYS

O 80.1 Thu 10:30 TRE/PHYS

Surface chemistry of silicate minerals at the atomic scale — LUCA LEZUO¹, ANDREA CONTI¹, ALEXANDER HOHENEDER¹, ELENA VANÍČKOVÁ², DOMITILLA ALOI¹, RAINER ABART³, FLORIAN MITTENDORFER¹, MICHAEL SCHMID¹, ULRIKE DIEBOLD¹, and GIADA FRANCESCHI¹ — ¹Inst. Appl. Phys., TU Wien, Austria — ²CEITEC, Brno, Czechia — ³Dept. Lithospheric Res., Uni Wien, Austria

Silicate minerals underpin key processes in geochemistry, atmospheric science, and materials technology, yet their atomic-scale surface chemistry remains insufficiently understood. Their intrinsic heterogeneity and electrical insulation have limited experimental characterization, leaving most mechanistic insight to simulations. Here, we extend the capabilities of noncontact atomic force microscopy (ncAFM) in ultrahigh vacuum to achieve atomic and chemical resolution on natural silicates such as muscovite mica,^{1,2} feldspar microcline³ and wollastonite.⁴ Our measurements provide direct evidence for processes central to mineral reactivity, such as ion hydration, ice nucleation, and carbonation reactions. They demonstrate that ncAFM affords fundamental insights previously restricted to theory and offer benchmark data to guide and challenge emerging computational models of mineral-gas interactions.

¹G.F. *et al.*, *Nat. Commun.* **14**, 208 (2023); ²G.F. *et al.*, *Faraday Discuss.* **249**, 84 (2024); ³G.F. *et al.*, *JPCL* **15**, 15 (2023); ⁴Conti *et al.*, *submitted* (2025).

O 80.2 Thu 11:00 TRE/PHYS

First Principles Investigations of Energy Dissipation Processes during Atom-Surface Collisions — NILS HERTL^{1,2} and REINHARD J. MAURER^{1,2,3} — ¹Department of Chemistry, University of Warwick, Coventry, UK — ²Department of Physics, University of Warwick, Coventry, UK — ³Department of Physics, University of Vienna, Vienna, Austria

H atom scattering experiments have emerged as a powerful tool for selectively probing the energy transfer mechanisms between adsorbate and surface, which are relevant for adsorption—the first elementary step in heterogeneous catalysis. This typically includes both phonon and electron excitation in the substrate. Yet, the latter is challenging to model with molecular dynamics because it requires simulation techniques that go beyond the Born-Oppenheimer approximation. In this talk, I will demonstrate how combining electronic structure theory, machine learning, and non-adiabatic molecular dynamics enables a quantitative study of energy transfer between H atoms and surfaces across diverse material classes. I will show that the computed energy loss spectra agree well with experimental findings, enabling detailed characterisation of individual energy transfer channels as well as processes that are experimentally inaccessible, such as adsorption. Based on these findings, I will present a conceptual framework that links adsorbate and surface electronic structure to the probability for non-adiabatic effects to occur in gas-surface collisions.

O 80.3 Thu 11:30 TRE/PHYS

Exchange-driven magnetoelastic coupling in a correlated itinerant ferromagnet — CAROLINA A. MARQUES¹, LUKE C. RHODES¹, WERONIKA OSMOLSKA¹, HARRY LANE¹, IZIDOR BENEDIČIĆ¹, MASAHIRO NARITSUKA¹, SIRI A. BERGE¹, ROSALBA FITTIPALDI², MARIATERESA LETTIERI², ANTONIO VECCHIONE², and PETER WAHL^{1,3} — ¹SUPA, School of Physics and Astronomy, University of St Andrews, UK — ²CNR-SPIN, c/o Università di Salerno, Italy — ³Physikalisches Institut, Universität Bonn, Germany

The electronic properties of materials are the result of the complex relationship between lattice and electronic degrees of freedom. In magnetic materials, exchange interactions leads to magnetoelastic cou-

pling, whose effect can be enhanced by the presence of electronic correlations. In the itinerant ferromagnet Sr₄Ru₃O₁₀, its magnetic and electronic properties are strongly influenced by electron correlations driven by Van Hove singularities close to the Fermi level. Here, we detect changes to the electronic structure, magnetic ground state and lattice in Sr₄Ru₃O₁₀ using scanning tunneling microscopy and spectroscopy (STM/STS). By switching between ferromagnetic and anti-ferromagnetic alignment of the magnetization of the surface and sub-surface layers, we study the impact of exchange interaction on the electronic structure and detect jumps in the interlayer spacing, revealing giant exchange magnetostriction in Sr₄Ru₃O₁₀. Our measurements reveal a direct link between exchange interaction, electronic and crystal structures, providing a platform to test theoretical descriptions of strongly correlated electron materials.

O 80.4 Thu 12:00 TRE/PHYS

Effect of atomic-scale defects on light-matter interaction in transition-metal dichalcogenides — VIBHUTI N. RAI, JUNYOUNG SIM, FLORIAN FAABER, SERGEY TRISHIN, NILS BOGDANOFF, PAUL WIECHERS, CAROLINE FIRSCHKE, TOM S. SEIFERT, TOBIAS KAMPFRATH, CHRISTIAN LOTZE, and KATHARINA J. FRANKE — Freie Universität Berlin, Department of Physics, Arnimallee 14, 14195 Berlin, Germany

Defects crucially affect the physical properties of (quasi-) two-dimensional materials, such as transition metal dichalcogenides (TMDCs). Here, by using THz scanning tunneling microscopy [1], we excite and detect long-range coherent in-plane shear and out-of-plane breathing modes on the surface of 2H-MoTe₂. We find that atomic-scale intrinsic defects influence their relative excitation efficiency. We attribute this response to local tip-induced band bending [2].

In the monolayer limit, where quantum confinement enhances defect sensitivity, we further show ultrafast charge modulation in defect sites of quasi-freestanding nanopatches of a monolayer MoS₂ on Au(111) driven by THz pulses. These insights into defect-mediated phonon excitation and charge transfer provide a pathway toward future ultrafast electronics.

[1] Cocker *et al.*, *Nature Photonics* **7**, 620-625 (2013)

[2] Rai *et al.* *arXiv:2506.08219v2* (2025)

O 80.5 Thu 12:30 TRE/PHYS

Topological Dirac Quasiparticles Tailored by Moiré Engineering — MAXIMILIAN ÜNZELMANN, ROMANA GANSER, MUTHU MASILAMANI, BEG MUHAMMET GELDIYEV, and FRIEDRICH REINERT — Exp. Physik VII and Würzburg-Dresden Cluster of Excellence ctd.qmat, Universität Würzburg, Germany

Moiré heterostructures have become a promising platform for tailoring electronic states in a highly controllable manner. The emergent superlattice potential gives rise to band gaps in the folded moiré band structure, which lead to a quenching of kinetic energy and thus increase of electron-electron interactions. Emergent flat bands have been observed in nano-focused angle-resolved photoemission spectroscopy (ARPES) experiments and demonstrated to trigger correlation-driven phenomena. Here, we go beyond the mere creation of flat bands and demonstrate that surface moiré engineering allows transforming a 'simple' epitaxial monolayer-substrate heterostructure into topological Dirac matter. In particular, using ARPES experiments, we will (i) prove the existence of one-dimensional Dirac fermions in the moiré-driven band structure, (ii) show that those are robustly protected by the emergent superlattice symmetry, and (iii) demonstrate how the entire mini-band structure can be controlled by epitaxial manners and sample temperature. Overall, this expands the potential of moiré materials by shifting the focus from almost exclusively flat bands to the creation of new, highly controllable Dirac quasiparticles.