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 Lezuo[1], Andrea Conti[1], Alexander Hoheneder[1], Elena Vaníčková[2], Domitilla Aloi[1], Rainer Abart[3], Florian Mittendorfer[1], Michael Schmid[1], Ulrike Diebold[1], and •Giada Franceschi[1] — [1]Inst. Appl. Phys., TU Wien, Austria — [2]CEITEC, Brno, Czechia — [3]Dept. 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 microcline[3] 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.

[1]G.F. *et al.*, *Nat. Commun.* **14**, 208 (2023); [2]G.F. *et al.*, *Faraday Discuss.* **249**, 84 (2024); [3]G.F. *et al.*, *JPCL* **15**, 15 (2023); [4]Conti *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] — [1]Department of Chemistry, University of Warwick, Coventry, UK — [2]Department of Physics, University of Warwick, Coventry, UK — [3]Department 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. Marques[1], Luke C. Rhodes[1], Weronika Osmolska[1], Harry Lane[1], Izidor Benedičič[1], Masahiro Naritsuka[1], Siri A. Berge[1], Rosalba Fittipaldi[2], Mariateresa Lettieri[2], Antonio Vecchione[2], and Peter Wahl[1,3] — [1]SUPA, School of Physics and Astronomy, University of St Andrews, UK — [2]CNR-SPIN, c/o Università di Salerno, Italy — [3]Physikalisches 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 coupling, whose effect can be enhanced by the presence of electronic correlations. In the itinerant ferromagnet $Sr_4Ru_3O_{10}$, 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 $Sr_4Ru_3O_{10}$ using scanning tunneling microscopy and spectroscopy (STM/STS). By switching between ferromagnetic and anti-ferromagnetic alignment of the magnetization of the surface and subsurface layers, we study the impact of exchange interaction on the electronic structure and detect jumps in the interlayer spacing, revealing giant exchange magnetostriction in $Sr_4Ru_3O_{10}$. 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-$MoTe_2$. 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 MoS_2 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, Begmuhammet 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.

O 81: Catalysis and surface reactions II

Time: Thursday 10:30–12:15 Location: TRE/MATH

O 81.1 Thu 10:30 TRE/MATH

Pd/Cu single atom alloys for selective alcohol dehydrogenation: from single crystalline to nanostructured model catalysts — •Philipp Alexander Fredersdorff[1], Jan Smyczek[1], Carsten Schroeder[1], Paul Froehlich[1], Paul Kohlmorgen[1], Stephan Appelfeller[2], Konstantin Neyman[3], and Swetlana Schauermann[1] — [1]Institute of Physical Chemistry, University Kiel, 24118 Kiel, Germany — [2]MAX IV Laboratory, Lund University, 22100 Lund, Sweden — [3]Departament de Ciència de Materials i Química Física & Institut de Química Teòrica i Computacional (IQTC-UB), Universitat de Barcelona, Barcelona 08028, Spain

Single-atom alloy (SAA) catalysts offer atomic-level control of selectivity, yet structure reactivity relationships in realistic systems remain insufficiently understood. Here, we report the first preparation of well-defined Pd/Cu single-atom alloy nanoparticles under UHV on Al2O3/NiAl(110) and investigate their properties using IRAS CO titration, STM, and TPD. Temperature-dependent Pd de-aggregation shows the same behaviour as on Pd/Cu(111), with optimal incorporation at 550 K. Both de-aggregated materials catalyze the non-oxidative dehydrogenation of butanol, but only the nanostructured Pd/Cu-NP SAA achieves 100 percent selectivity, completely suppressing CO formation. A Pd-coverage-dependent analysis reveals that cluster formation rapidly decreases aldehyde selectivity on single-crystal Pd/Cu(111), whereas the newly developed nanostructured SAA catalysts maintain full selectivity across a wide Pd range.