TT 49: Correlated Electrons: Charge Order

Time: Wednesday 10:45–12:45 Location: HSZ/0101

TT 49.1 Wed 10:45 HSZ/0101

Charge density wave and superconductivity interplay in 2H-$TaSe_2$ — •Yuliia Tymoshenko[1], Amir-Abbas Haghighirad[1], Rolf Heid[1], Gaston Garbarino[2], Luigi Paolasini[2], and Frank Weber[1] — [1]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [2]European Synchrotron Radiation Facility, 71 avenue des Martyrs, CS 40220, Grenoble 38043, France

The suppression of an ordered state is often discussed as a pathway to enhancing superconducting (SC) transition temperatures. Transition-metal dichalcogenides (TMDs), where both charge-density-wave (CDW) order and superconductivity arise from electron-phonon coupling, offer an ideal platform to study this interplay.

We performed high-pressure single-crystal X-ray diffraction (XRD) and inelastic X-ray scattering (IXS) on 2H-$TaSe_2$ and traced the evolution of its CDW superstructure and soft phonon mode over a broad temperature-pressure range. Our measurements show that the suppression of CDW order remains continuous down to low temperatures, demonstrating the persistence of a second-order phase transition, which is a necessary prerequisite for a CDW-related quantum-critical scenario. These findings refine the understanding of how CDW order collapses under pressure and how this behavior relates to the reported maximum superconducting transition temperature near 20 GPa.

Overall, 2H-$TaSe_2$ emerges as a controlled model system for investigating the interplay between CDW order, lattice dynamics, and superconductivity.

TT 49.2 Wed 11:00 HSZ/0101

Dynamics of CDW puddles in bulk 2H-$NbSe_2$ — •Shreya Kumbhakar[1,2], Marina Esposito[3], Anjan Kumar N M[1], Sushmita Chandra[4], Claudia Felser[4], Kornelius Nielsch[1,2], Nicola Poccia[2,3], Stefan Kaiser[1], and Golam Haider[2] — [1]TU Dresden — [2]IFW Dresden — [3]U. Naples — [4]MPI CPfS

In complex materials, incommensurate charge-density-wave (CDW) is often formed from local commensurate domains or puddles. Measuring the dynamics of these puddles, we probe the effect of lattice pinning, electronic correlations and disorder on emergent phases. Raman scattering reveals a Fano lineshape of the CDW amplitude mode, indicating strong coupling between the interlayer shear vibration and the CDW order. Time-resolved reflectivity shows a coherent overdamped oscillation below the CDW transition temperature, indicating a new low-frequency hybrid phonon-CDW amplitude mode around 0.15 THz. This we identify as the CDW puddle emerging from the strong Fano coupling. Our measurements further reveal a transition at 14 K, pointing to a possible crossover of the dominant commensuration order of these puddles. These results highlight how the layered structure affects the CDW order, which is crucial for the design and understanding of novel vdW heterostructures.

TT 49.3 Wed 11:15 HSZ/0101

Electronic band gap tuning of interchain phonon transport in $Ta_2Ni(S_xSe_{1-x})_5$ — Yuan-Shan Zhang[1], Masahiko Isobe[1], Hidenori Takagi[1,2,3], and •Dennis Huang[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Germany — [3]National Institute for Materials Science, Tsukuba, Japan

The dual electronic and structural characters of the 326 K transition in the quasi-one-dimensional compound Ta_2NiSe_5 continues to inspire heated discussion as to the origin of its primary driving force. The current state of affairs may be best summarized as a three-party debate, in which electron-hole interactions (excitonic insulator), electron-lattice coupling (hybridization gap), and "instrinsic" lattice effects are all championed to play some role. The isostructural compound Ta_2NiS_5 should serve as a valuable foil for better understanding Ta_2NiSe_5, as substitution of Se for S enlarges the single-particle electronic band gap, which diminishes the role of electronic degrees of freedom and greatly reduces the transition temperature. Here, we report thermal transport measurements that probe the interchain phonon conductivity of $Ta_2Ni(S_xSe_{1-x})_5$. A soft-phonon anomaly observed in the Se-rich compounds is absent in the S-rich compounds, implying the crucial role of electronic (excitonic and hybridization-gap) fluctuations that couple to the lattice and boost the structural transition temperature.

TT 49.4 Wed 11:30 HSZ/0101

Doping tunable charge density waves in misfit layer compounds — •Hugo Le Du[1], Ludovica Zullo[2], Justine Cordiez[3], Robin Salvatore[1], Daniel Schmieg[1], Giovanni Marini[4], François Debbontridder[1], Marie Hervé[1], Shunsuke Sasaki[3], Florent Pawula[3], Etienne Janod[3], Matteo Calandra[4], Laurent Cario[3], and Tristan Cren[1] — [1]Institut des Nanosciences de Paris, Sorbonne Université, Paris, France — [2]Julius-Maximilians-Universität Würzburg, Würzburg, Germany — [3]Institut des Matériaux de Nantes, Nantes, France — [4]University of Trento, Italy

Misfit layer compounds are van der Waals heterostructures formed by stacking transition metal dichalcogenide (TMD) and monochalcogenide layers. Theoretically, charge transfer from monochalcogenide to TMD layers results in significant doping. Adjusting the monochalcogenide composition enables precise control over TMD doping levels. We show via scanning tunneling microscopy (STM) that in $(La_xPb_{1-x}Se)1.14(NbSe_2)_2$, the $NbSe_2$ Fermi level shifts from 0.0 eV to 0.3 eV by varying La content. Combining STM with DFT calculations, we demonstrate that $NbSe_2$ transitions from the conventional 3×3 CDW state to alternative configurations at higher doping. Superconducting properties also change, offering a novel platform to explore the interplay between superconductivity and charge density waves.

TT 49.5 Wed 11:45 HSZ/0101

Coherent amplitude response in the excitonic insulator $Ta_2Pd_3Te_5$ — •Anjan Kumar Naralapura Manohara[1], Shuhan Wang[1], Snehashish Chatterjee[2], Chandra Shekhar[2], Claudia Felser[2], and Stefan Kaiser[1] — [1]Institute of Solid State and Materials Physics, TU dresden — [2]Topological Quantum Chemistry Group, Max Planck Institute for Chemical Physics of Solids, Dresden

The excitonic insulator represents a fascinating electronic phase in which bound electron-hole pairs condense into a macroscopic quantum state. The layered compound $Ta_2Pd_3Te_5$ has recently emerged as a compelling platform for exploring this elusive phase. A hallmark of such condensate is the presence of collective excitations analogous to the Higgs (amplitude) and Goldstone (phase) modes in superconductors. In this work, we present the experimental fingerprint of a coherent amplitude response in the excitonic insulator phase of $Ta_2Pd_3Te_5$. Through non-degenerate pump-probe spectroscopy, we identify three low frequency A1g phonons that show strong coupling to the excitonic condensate. We characterise these modes as a function of temperature and excitation fluence to reveal their link to the emergence and dynamics of the excitonic condensate.

TT 49.6 Wed 12:00 HSZ/0101

Doping-tunable charge ordering in semiconducting single-layer Cr_2Se_3 — •Sisheng Duan and Miguel Ugeda — Donostia International Physics Center, Paseo Manuel de Lardizábal 4, 20018 San Sebastián, Spain

The charge density wave (CDW), a charge ordering phase, offers a valuable framework for exploring electron-electron interactions, electron-phonon coupling, and quantum phase transitions. In CDW materials, carrier density substantially influences the ground state, typically altered through foreign ion doping and investigated at macro- or mesoscopic scales via photoemission or transport techniques. However, atomic-scale visualization, particularly in doped CDW systems without foreign ions, remains rare. Here, we present real-space observation of doping-tunable granular charge ordering using scanning tunneling microscopy in semiconducting single-layer Cr_2Se_3, a group VIB transition metal chalcogenide. Observations of lattice distortion, bandgap modulation at the Fermi energy, and STM contrast inversion at low temperatures indicate a charge ordering origin. The semiconducting nature of Cr_2Se_3 enables charge ordering modulation through doping: Hole doping suppresses it, whereas electron doping alters the pattern, yielding a periodic $3\sqrt{3} \times 3\sqrt{3}$ CDW phase. This tunable charge ordering in a group VIB TMC advances the understanding of charge doping and ordering interactions in two-dimensional materials.

TT 49.7 Wed 12:15 HSZ/0101

On the origin of charge density waves as an emergent phenomenon from the electron-phonon interactions in $ZrTe_3$

— •Raghottam M Sattigeri[1,2], Niccolò Mignani[1], Claudia Dallera[1], Ettore Carpene[1], Simona Achilli[2], and Alberto Crepaldi[1] — [1]Physics Department, Politecnico di Milano, Milano, Italy — [2]Physics Department, University of Milan, Milan, Italy

Charge density ordering is not elusive in electronic structures which are highly anisotropic, thus indicating a strong electron-phonon (e-ph) interaction which drives such phenomenon. There has been an active debate on the origin of such ordering in two-dimensional transition metal dichalcogenides, however, similar investigations for bulk materials are scarce. It is evident from experiments that, quasi one-dimensional crystal structure $ZrTe_3$ exhibits stable modulations with long-range ordering which facilitates the system to host charge density waves (CDW). We address and investigate thoroughly the origin of CDW in bulk $ZrTe_3$ using density functional theory based first-principles calculations. We analyze the role of electronic instability and e-ph coupling, respectively, as possible mechanisms for the formation of CDW. From our calculations we were able to identify a peak in the the Lindhard response function and strong e-ph interactions suggesting that, both, the electronic and phononic contributions have a role in the process of CDW ordering in $ZrTe_3$.

TT 49.8 Wed 12:30 HSZ/0101

Controlling metastable charge-ordered states in δ-$Ag_{2/3}V_2O_5$

— •Masahiko Isobe[1], Taisei Kubo[2], Naoyuki Katayama[2], and Robert E. Dinnebier[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [2]Department of Applied Physics, Nagoya University, Nagoya 464-8603, Japan

Vanadium bronzes have attracted much interest as a playground of various quantum phenomena. They are essentially mixed valent oxides where metallic conductivity and novel phenomena with spin, charge and orbital degrees of freedom can be exhibited. Recently we have investigated the delta-phase of vanadium bronze, focusing on the phase transition in δ-$Ag_{2/3}V_2O_5$ which shows characteristic supercooling effects. The structure consists of double trellis layer formed by edge/corner-shared VO_6 octahedra and Ag ions located between the layers. We have observed the phase transition at around 230 K accompanied by jumps of magnetic susceptibility and resistivity. Structural analysis of the low-temperature triclinic phase reveals that Ag ion order and Vanadium dimer formation. Below the transition temperature the magnetic susceptibility shows a broad maximum around 110 K followed by spin gap behavior. We conclude that the phase transition in δ-$Ag_{2/3}V_2O_5$ is a charge order into V^{4+} and V^{5+} induced by Ag ion order. The V^{4+} ions form dimers with the spin-gapped ground state. Also it can be super-cooled down to the lowest temperature by rapid cooling.