

## TT 39: Correlated Electrons: Charge Order

Time: Wednesday 9:30–12:15

Location: H 3025

TT 39.1 Wed 9:30 H 3025

**Kinetic theory and collective modes in the charge-density-wave phase of  $K_{0.3}MoO_3$**  — VIKTOR HAHN, ●MAX O. HANSEN, and PETER KOPIETZ — Goethe University, Frankfurt am Main, Germany

Initiated by recent measurements of collective modes in the charge-density-wave (CDW) state of the electronically quasi-one-dimensional material  $K_{0.3}MoO_3$  [1], we present a theoretical study of amplitude and phase modes in the incommensurate CDW state. For this purpose we formulate a kinetic theory using an expansion in powers of connected equal-time correlations. Our linearized kinetic equations for the CDW order parameter have the same form as the phenomenological equation of motion obtained within a time-dependent Ginzburg-Landau approach. Frequencies and damping coefficients for the amplitude and phase modes in the CDW state can be extracted numerically or directly from the linearized kinetic equations. We find that the damping is strongly enhanced when the temperature approaches the critical temperature from below, in agreement with recent experiments [1].

[1] K. Warawa, N. Christophel, S. Sobolev, J. Demsar, H. G. Roskos, M. D. Thomson, Phys. Rev. B **108** (2023) 045147.

TT 39.2 Wed 9:45 H 3025

**Kohn-Luttinger-like mechanism for charge density waves** — ●HANNES BRAUN — Max Planck Institute for Solid State Research, Stuttgart, Germany

We propose a Kohn-Luttinger-like mechanism for charge density waves with higher angular momentum in correlated electron systems. The mechanism describes an instability in the particle-hole direct channel, which emerges due to the feedback from the particle-hole crossed channel. Like in the original Kohn-Luttinger mechanism for superconductivity, the separation of vertex corrections in different lattice harmonics is the key for getting attractive components out of an initially repulsive interaction. We provide numerical as well as analytical arguments for the realisation of this mechanism in the triangular lattice Hubbard model with higher  $SU(N)$  symmetry, which can be implemented, e.g., in cold atomic gases or moiré bilayers of transition metal dichalcogenides.

TT 39.3 Wed 10:00 H 3025

**Elastoresistance of the charge-density-wave material  $NbSe_2$**  — ●MAIK GOLOMBIEWSKI, TIANYI XU, SIMON KNUDSEN, TESLIN R. THOMAS, SVEN GRAUS, ANDREAS KREYSSIG, and ANNA E. BÖHMER — Lehrstuhl für Experimentalphysik IV, Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum

Mono- and diselenides such as FeSe, FeSe<sub>2</sub> and NbSe<sub>2</sub> display many interesting and diverse properties. For example, FeSe is a well-known nematic superconductor, whereas NbSe<sub>2</sub> exhibits superconductivity below  $T_c = 7.2$  K and a charge-density-wave (CDW) phase below  $T_{CDW} = 32$  K. Optimizing growth parameters, we have grown large and homogeneous single crystals of FeSe, FeSe<sub>2</sub> and NbSe<sub>2</sub> via chemical vapor transport. Samples were characterized via x-ray diffraction, energy-dispersive x-ray spectroscopy and electrical resistance. In particular, we have determined the change of electrical resistance of NbSe<sub>2</sub> under strain, i.e., its elastoresistance, around  $T_{CDW}$ , using piezostacks and a cryogenic strain cell. A subtle anomaly in the linear elastoresistance at  $T_{CDW}$  is observed. The effect of large elastic strains on the resistance will also be discussed.

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TT 39.4 Wed 10:15 H 3025

**Giant circular dichroism induced by electronic chirality in  $TiSe_2$**  — QIAN XIAO<sup>1</sup>, ●OLEG JANSON<sup>2</sup>, SONIA FRANCOUAL<sup>3</sup>, QINGZHENG QIU<sup>1</sup>, QIZHI LI<sup>1</sup>, SHILONG ZHANG<sup>1</sup>, WU XIE<sup>3,4</sup>, PABLO BERECIARTUA<sup>3</sup>, JEROEN VAN DEN BRINK<sup>2,5,6</sup>, JASPER VAN WEZEL<sup>6</sup>, and YINGYING PENG<sup>1,7</sup> — <sup>1</sup>Peking University, Beijing, China — <sup>2</sup>Institute for Theoretical Solid State Physics, Leibniz IFW Dresden, Germany — <sup>3</sup>DESY, Hamburg, Germany — <sup>4</sup>Zhejiang University, Hangzhou, China — <sup>5</sup>Würzburg-Dresden Cluster of Excellence ct.qmat, Germany — <sup>6</sup>Institute for Theoretical Physics, University of Amsterdam, The Netherlands — <sup>7</sup>Collaborative Innovation Center of Quantum Matter, Beijing, China

The quasi-2D van-der-Waals material  $1T-TiSe_2$  is known for its well-studied transition into a commensurate  $2\times 2\times 2$  charge density wave (CDW) state. Several experimental and theoretical studies suggested that the charge order may be chiral, yet no bulk measurement so far provided direct evidence for intrinsic broken inversion symmetry and chirality. In a resonant elastic x-ray scattering (REXS) experiment, we observe giant circular dichroism up to  $\sim 40\%$  at a Bragg peak forbidden in the centrosymmetric CDW structure. By performing first-principles calculations for the earlier proposed chiral structural model, we find excellent quantitative agreement with the experimental azimuthal angle dependence for different polarizations. In this way, we accurately estimate the magnitude of the inversion-breaking distortion and confirm that bulk  $1T-TiSe_2$  has chiral electronic order.

TT 39.5 Wed 10:30 H 3025

**Quenched exciton condensate in  $TiSe_2$  probed by surface-sensitive electron diffraction** — ●FELIX KURTZ<sup>1</sup>, TIM NIKLAS DAUWE<sup>1</sup>, SERGEY V. YALUNIN<sup>1</sup>, GERO STORECK<sup>1</sup>, JAN GERRIT HORSTMANN<sup>2</sup>, HANNES BÖCKMANN<sup>1</sup>, and CLAUS ROPERS<sup>1,3</sup> — <sup>1</sup>Max Planck Institute for Multidisciplinary Sciences, D-37077 Göttingen — <sup>2</sup>Department of Materials, ETH Zurich, CH-8093 Zürich — <sup>3</sup>4th Physical Institute, University of Göttingen, D-37077 Göttingen

Charge-density waves (CDWs) are intriguing correlated phenomena, arising from strong couplings among electrons or between electronic and lattice degrees of freedom. In particular,  $TiSe_2$  showcases signs of both excitonic condensation and a Peierls mechanism driving the phase transition to the CDW state below 200 K. Jointly occurring in equilibrium, time-resolved studies are capable of disentangling these contributions [1]. Here, we employ ultrafast low-energy electron diffraction (ULEED) [2] to trace the structural order parameter in the surface layer of  $TiSe_2$  after photoexcitation. We identify a low fluence threshold similar to other time-resolved works, which allows us to directly quantify the excitonic contribution to the total lattice distortion [3]. It is completely quenched at the threshold, and from the persisting distortion we estimate a 30:70 split of the structural order parameter into excitonic and Peierls contributions. Our findings highlight the strengths of ultrafast structural probing with monolayer sensitivity offered by ULEED.

[1] M. Porer et al., Nat. Mater. **13** (2014) 857.

[2] G. Storeck et al., Struct. Dyn. **7** (2020) 034304

[3] F. Kurtz et al., under review (2023)

## 15 min. break

TT 39.6 Wed 11:00 H 3025

**Comparative optical study of the CDW states in various  $TaS_2$  polymorphs** — ●RENJITH MATHEW ROY<sup>1</sup>, MAXIM WENZEL<sup>1</sup>, SUDIP PAL<sup>1</sup>, VICKY HASSE<sup>2</sup>, CLAUDIA FELSER<sup>2</sup>, ARTEM V. PRONIN<sup>1</sup>, and MARTIN DRESSEL<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany — <sup>2</sup>Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany

We report the temperature-dependent optical conductivity of the bulk transition-metal dichalcogenides  $4H_b-TaS_2$ ,  $2H-TaS_2$ , and  $6R-TaS_2$ , studied in a broad energy range from 10 meV to 2.5 eV. These kagome-structured compounds possess a charge density wave (CDW) state below  $T_{CDW} = 22, 75,$  and  $305$  K, respectively. The presence of coexisting superconductivity and possible chiral CDW order, as well as the occurrence of topological flat bands in various polymorphs of  $TaS_2$ , fueled the recent interest in their studies [1-4]. In all three compounds, we observe a common interband response above 100 meV and distinguishable signatures of band reconstruction below  $T_{CDW}$ . Our compassion provides a broader picture of the CDW-formation mechanism via detecting the energy gaps and possible charge localization, emerging in these quasi-2D systems.

[1] A. Ribak et al., Sci. Adv. **6**, eaax9480 (2020)

[2] S. Pal et al., Phys. B: Cond. Mat. **669** (2023) 415266.

[3] I. Guillaumon et al., New J. Phys. **13** (2011) 103020.

[4] J. M. Lee et al., Phys. Rev. Lett. **124** (2020) 137002.

TT 39.7 Wed 11:15 H 3025

**Ultrafast dynamics in  $(TaSe_4)_2I$  triggered by valence and core-level excitation** — ●WIBKE BRONSCH<sup>1</sup>, MANUEL TUNIZ<sup>2</sup>,

GIUSEPPE CRUPI<sup>2</sup>, MICHELA DE COL<sup>2</sup>, DENNY PUNTEL<sup>2</sup>, DAVIDE SORANZIO<sup>2</sup>, ALESSANDRO GIAMMARINO<sup>2</sup>, MICHELE PERLANGELI<sup>2</sup>, HELMUTH BERGER<sup>3</sup>, DARIO DE ANGELIS<sup>1</sup>, DANNY FAINOZZI<sup>1</sup>, ETTORE PALTANIN<sup>2</sup>, STEFANO PELLI CRESI<sup>1</sup>, GABOR KURDI<sup>1</sup>, RICCARDO MINCIGRUCCI<sup>1</sup>, LAURA FOGLIA<sup>1</sup>, FULVIO PARMIGIANI<sup>1</sup>, FILIPPO BENCIVENGA<sup>1</sup>, and FEDERICO CILENTO<sup>1</sup> — <sup>1</sup>Elettra - Sincrotrone Trieste S.C.p.A., Strada Statale 14, km 163.5, Trieste, Italy — <sup>2</sup>Dipartimento di Fisica, Università degli Studi di Trieste, 34127 Trieste, Italy — <sup>3</sup>Institute of Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

Dimensionality plays a key role for the emergence of ordered phases like charge-density-waves, that in turn can couple to and modulate the topological properties of matter. In this work, we study the out-of-equilibrium dynamics of the paradigmatic quasi-one-dimensional material (TaSe<sub>4</sub>)<sub>2</sub>I, that exhibits a transition into an incommensurate charge-density-wave (CDW) phase when cooled down just below room temperature, at  $T_{CDW} = 263$  K. We make use of both optical laser and free-electron laser (FEL) based time-resolved spectroscopies in order to study the effect of a selective excitation of the material on the charge-density-wave phase, by probing the near-infrared/visible optical properties both along and perpendicularly to the direction of the charge-density-wave [1].

[1] W. Bronsch et al., Faraday Discuss. 237 (2022) 40.

TT 39.8 Wed 11:30 H 3025

**Substrate tuning of transition temperature in thin flakes of the excitonic insulator candidate Ta<sub>2</sub>NiSe<sub>5</sub>** — •YUANSHAN ZHANG<sup>1</sup>, ZICHEN YANG<sup>1</sup>, DENNIS HUANG<sup>1</sup>, MATTEO MINOLA<sup>1</sup>, CHUANLIAN XIAO<sup>1</sup>, MASAAHIKO ISOBE<sup>1</sup>, BERNHARD KEIMER<sup>1</sup>, and HIDENORI TAKAGI<sup>1,2,3</sup> — <sup>1</sup>Max Planck Institute for Solid State Research, Stuttgart, Germany — <sup>2</sup>Department of Physics, University of Tokyo, Japan — <sup>3</sup>Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Germany

The nature of the transition in Ta<sub>2</sub>NiSe<sub>5</sub> to an insulator around 326 K remains an active debate. The discussion focuses on whether the transition is predominantly structural, as evidenced by an orthorhombic-to-monoclinic lattice transition, or electronic/excitonic, as understood through the interplay between the energy gap and excitonic binding energy. We have separated electron and phonon effects by employing thin Ta<sub>2</sub>NiSe<sub>5</sub> flakes on both conducting Au and insulating Al<sub>2</sub>O<sub>3</sub> substrates. Polarized Raman spectroscopy indicates that the lattice transition is largely unchanged in flakes as thin as 3 nm on Al<sub>2</sub>O<sub>3</sub>, whereas it is reduced by nearly 100 K on Au. Model analysis reveals that the underlying electronic excitation in the latter does not exhibit an excitonic instability. We discuss how the conducting substrate influences an excitonic insulator. Our findings demonstrate that the transition in Ta<sub>2</sub>NiSe<sub>5</sub> is charge-sensitive and cannot be attributed solely to a lattice instability. The electronic/excitonic instability appears to have an energy scale of approximately 100 K.

TT 39.9 Wed 11:45 H 3025

**Interlayer coupling between two charge density waves in 4H<sub>b</sub>-TaS<sub>2</sub>** — •CAROLINA A. MARQUES<sup>1</sup>, BERK ZENGIN<sup>1</sup>, ALEŠ CAHLÍK<sup>1</sup>, DANYANG LIU<sup>1</sup>, HELMUTH BERGER<sup>2</sup>, ANA AKRAP<sup>3</sup>, and FABIAN D. NATTERER<sup>1</sup> — <sup>1</sup>Department of Physics, University of Zurich, Switzerland — <sup>2</sup>Institute of Condensed Matter Physics, École Polytechnique Fédérale de Lausanne, Switzerland — <sup>3</sup>Department of Physics, University of Fribourg, Switzerland

The van der Waals material 4H<sub>b</sub>-TaS<sub>2</sub> is a superlattice of alternating layers with 1H and 1T coordination structures. The charge density waves (CDW) of each individual layer persist within the bulk of the material, and the superconducting temperature is enhanced compared to the pristine 2H-TaS<sub>2</sub>. Here, we use scanning tunneling microscopy and quasiparticle interference (QPI) to investigate the interaction between adjacent CDWs, and with the superconducting state. We identify a weakly dispersing band from QPI on the 1T surface and find domains with different orientations of the CDW, which change the observed Moiré patterns at the surface and the energy onset of the weakly dispersing band.

TT 39.10 Wed 12:00 H 3025

**The pressure-induced charge-density-wave transition in CeTe<sub>3</sub> probed by time-resolved collective mode spectroscopy** — •PRIYANKA YOGI<sup>1</sup>, C. VARDHAN KOTYADA<sup>1</sup>, J. TAUCH<sup>2</sup>, H. SCHÄFER<sup>2</sup>, M. OBERGFELL<sup>1,2</sup>, D. DOMINKO<sup>1</sup>, A. PASHKIN<sup>3</sup>, and JURE DEMSAR<sup>1</sup> — <sup>1</sup>Institute of Physics, Johannes Gutenberg University Mainz, 55128 Mainz, Germany — <sup>2</sup>Department of Physics, University of Konstanz, Germany — <sup>3</sup>Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

We use time-resolved optical spectroscopy to study pressure-induced charge-density-wave (CDW) phase transition in a prototype CDW system CeTe<sub>3</sub> (T<sub>3</sub> = 540 K at ambient pressure [1]). Photoinduced reflectivity traces at 300 K and ambient pressure reveal the presence of numerous oscillatory modes with frequencies between 1.2 and 4 THz. The modes display either softening or hardening as a function of pressure, yet all disappear above 5 GPa. Moreover, these modes are quenched above critical photoexcitation density. We compare the pressure and excitation density dependent mode parameters with the available temperature, chemical- and hydrostatic-pressure dependent Raman data on RTe<sub>3</sub> series [1,2]. We show that all modes are CDW amplitude modes, a result of linear coupling between the electronic order and normal-state phonons at the CDW wavevector [3]. Thus, the studies reveal a pressure-induced transition into the metallic state taking place in CeTe<sub>3</sub> at the critical pressure of 5 GPa at 300 K.

[1] K. Yumigeta et al., APL Mater. 10 (2022) 111112.

[1] M. Lavagnini et al., Phys. Rev. B 78 (2008) 201101.

[2] K. Warawa et al., Phys. Rev. B 108 (2023) 045147.