TT 51: Correlated Electrons: Charge Order

Time: Thursday 15:00–17:30 Location: HSZ 103

TT 51.1 Thu 15:00 HSZ 103

The zoo of magnetic states in the 2D Hubbard model — •Robin Scholle, Pietro Bonetti, Demetrio Vilardi, and Walter Metzner — MPI FKF Stuttgart

We use real-space Hartree-Fock theory to construct a magnetic phase diagram of the two-dimensional Hubbard model as a function of temperature and doping. We are able to detect various spin- and charge order patterns including Néel, stripe and spiral order without biasing the system towards one of them. For an intermediate interaction strength we predominatly find Néel order close to half-filling, stripe order for low temperatures or large doping, and an intermediate region of spiral order.

I will give a short summary of the method followed by a presentation of our current results and an outlook for possible further applications.

TT 51.2 Thu 15:15 HSZ 103

Effect of higher-order van Hove singularity on the formation of spin density waves — Alkistis Zervou[1], Garry Goldstein[2], Joseph Betouras[1], and •Dmitry Efremov[3] — [1]Department of Physics and Centre for the Science of Materials, Loughborough University, Loughborough LE11 3TU, UK. — [2]Physics Department, Boston University, Boston MA 02215, USA — [3]Leibniz Institute for Solid State and Materials Research Dresden, Helmholtzstrasse 20, D-01069 Dresden, Germany.

Van-Hove singularities in the density of states, which occur due to Lifshitz transitions in electronic band structures, affect different types of ordering in quantum materials. In addition to the usual Van Hove singularities, there are higher-order Van Hove singularities (HOVHS) with DOS divergence according to the power law. We find that the spin wave density and charge density of the phase formation can be enhanced by the presence of a singularity depending on the strength of certain interactions, with the critical temperature increasing by orders of magnitude. We discuss the application of our findings to various experimental systems such as Sr3Ru2O7.

15 min. break

TT 51.3 Thu 15:45 HSZ 103

Kinetic theory of charge-density waves — •Viktor Hahn and Peter Kopietz — Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Strasse 1, 60438 Frankfurt, Germany

We present a theoretical study of the dynamics of the collective amplitude and phase modes in the charge-density wave (CDW) state of the electronically quasi one-dimensional material $K_{0.3}MoO_3$ (blue bronze). For this purpose we formulate a kinetic theory using the method of expansion in connected equal-time correlations. Our kinetic equations for the CDW order parameter has the same form as the phenomenological equation of motion obtained within a time-dependent Ginzburg-Landau approach. From the numerical solution of our kinetic equations we extract the frequencies and the damping of the collective amplitude and phase modes in the CDW state. We find that the damping is strongly enhanced when the temperature approaches the critical temperature from below, in agreement with recent experiments.

TT 51.4 Thu 16:00 HSZ 103

Collective modes in the quasi one-dimensional charge-density wave material blue bronze — •Max Oberon Hansen — Goethe University, Frankfurt am Main, Germany

We calculate the spectrum of collective modes (amplitude, phase, phonon, and plasmon) in the charge-density wave state of the quasi-one dimensional metal $K_{0.3}MoO_3$, named blue bronze. Using a functional integral approach we derive effective actions for the different types of collective modes in Gaussian approximation and compare our results with experiments. Our approach emphasizes the role of acoustic phonons to guarantee that the phase mode remains gapless in the presence of long-range Coulomb interactions.

TT 51.5 Thu 16:15 HSZ 103

Lattice instability in charge-frustrated CsW_2O_6 — •Pascal Reiss[1], Peter Wochner[1], Armin Schulz[1], Jürgen Nuss[1], Masahiko Isobe[1], and Hidenori Takagi[1,2,3] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Germany — [3]Department of Physics, The University of Tokyo, Bunkyo, Tokyo, Japan

The transition metal compound CsW_2O_6 represents an intriguing example of a pyrochlore structure at quarter filling. Starting from a bad metal with a nominal $W^{5.5+}$ oxidation state, the system suffers a metal-to-insulator transition around $T_c \approx 215\,K$. Here, a breathing distortion leads to the formation of regular molecular W_3 trimers with 2 localised electrons each, and a remaining W^{6+} site devoid of $5d$ electrons [1]. However, the origin of the transition as well as the electronic nature of the low-temperature phase remain unclear [2].

To elucidate the origin of the 215 K transition, we will present our recent structural investigations and transport measurements on CsW_2O_6 conducted under high pressures, where we uncover another structural instability, distinct from the ambient pressure one.

[1] Y. Okamoto et al., Nat. Commun. 11 (2020)
[2] N. Nakai and C. Hotta, Nat. Commun. 13 (2022)

TT 51.6 Thu 16:30 HSZ 103

Pressure-induced stabilization mechanism of molecular orbital crystals in $IrTe_2$ — •Tobias Ritschel[1], Quirin Stahl[1], Maximilian Kusch[1], Gaston Garbarino[2], Volodymyr Svitlyk[2], Mohamed Mezouar[2], Junjie Yang[3], Sang-Wook Cheong[4], and Jochen Geck[1] — [1]Institute of Solid State and Materials Physics, TU Dresden, 01069 Dresden, Germany — [2]ESRF, Grenoble, France — [3]New Jersey Institute of Technology, Newark, New Jersey 01702, USA — [4]Rutgers, New Jersey, USA

Doped $IrTe_2$ is considered a platform for topological superconductivity and therefore receives currently a lot of interest. In addition, the superconductivity in these materials exists in close vicinity to electronic order and the formation of molecular orbital crystals, which we explore here by means of high-pressure single crystal x-ray diffraction in combination with density functional theory. Our crystallographic refinements provide detailed information about the structural evolution as a function of applied pressure up to 42 GPa. Using this structural information for density functional theory calculations, we show that the local multicenter bonding in $IrTe_2$ is driven by changes in the Ir-Te-Ir bond angle. When the electronic order sets in, this bond angle decreases drastically, leading to a stabilization of a multicenter molecular orbital bond. This unusual local mechanism of bond formation in an itinerant material provides a natural explanation for the different electronic orders in $IrTe_2$. It further illustrates the strong coupling of the electrons with the lattice and is most likely relevant for the superconductivity in this material.

TT 51.7 Thu 16:45 HSZ 103

Lifshitz transition at the onset of superconductivity from mismatched nesting in $TiSe_2$ — •Roemer Hinlopen[1], Owen Moulding[1,2], Felix Flicker[3], Charles Sayers[4], Enrico Da Como[4], Jasper van Wezel[5], and Sven Friedemann[1] — [1]University of Bristol, UK — [2]Institut Néel, Grenoble, France — [3]Cardiff University, UK — [4]University of Bath, UK — [5]University of Amsterdam, The Netherlands

Fermi surface reconstructions and topological (Lifshitz) transitions can have a profound effect on the electronic ground state of a metal. For example, re-entrant superconductivity (SC) in URhGe may be due to the appearance of a small pocket [1], whereas in Bechgaard salts [2] and doped $BaFe_2As_2$ [3] the appearance of large pockets from mismatched nesting may give rise to SC within the magnetic phase.

Here, we report quantum oscillation measurements and DFT calculations under pressure in the prototypical charge density wave (CDW) compound $TiSe_2$. We observe the emergence of new Fermi surface pockets at 2 GPa within the CDW arising as a result of mismatched nesting. This Lifshitz transition coincides with the emergence of superconductivity [4], suggesting an intimate link between SC and the presence of these Fermi pockets similar to $BaFe_2As_2$. This suggests that SC in $TiSe_2$ might be of extended $s^{\pm}$-wave character - the first such case in a CDW system.

[1] Yelland, Nat. Phys. 7, 890 (2011)
[2] Bourbonnais, C. R. Physique 12, 532 (2011)
[3] Liu, Nat. Phys. 6, 419 (2010)
[4] Kusmartseva, PRL 103, 236401 (2009)

TT 51.8 Thu 17:00 HSZ 103

Spin stripe fluctuations in antiferromagnetic $Pr_{2-x}Sr_xNiO_{4+\delta}$ — •Avishek Maity[1], Rajesh Dutta[2,3], and Werner Paulus[4] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, 85747 Garching, Germany — [2]Institut für Kristallographie, RWTH Aachen Universität, 52066 Aachen, Germany — [3]Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), 85747 Garching, Germany — [4]ICGM, Univ. Montpellier, CNRS, ENSCM, Montpellier, France

Spin and charge stripe correlations and their dynamics have been well explored in the ordered state of $RE-$based 214-nickelates for last 3 decades. In this regards, what remains less explored is the fluctuating state of the spin stripes from which the long-range spin stripes develop on cooling. In this talk, we present our recent inelastic neutron scattering study of the low energy spin stripe fluctuations in $Pr_{2-x}Sr_xNiO_{4+\delta}$ with magnetic incommensurability $\epsilon = 0.33$ above the spin stripe ordering temperature $T_{so} = 190$ K [1]. The spin stripe fluctuations measured at the at the incommensurate wave vector show a non-dispersive character with no detectable anisotropy persisting up to a maximum energy 10 meV, and strongly suppressed already below the charge stripe ordering temperature $T_{co} = 255$ K. Our results clearly indicate the presence of static charge stripe order is essential for the spin stripe fluctuations in 214-type nickealtes.

[1] A. Maity *et al.*, Phys. Rev. B 106, 024414 (2022)

TT 51.9 Thu 17:15 HSZ 103

Glass-like transitions in the frustrated charge system θ-$(BEDT\text{-}TTF)_2MM'(SCN)_4$ (MM' = CsZn, CsCo, and RbZn) revealed by thermal expansion measurements — •Yohei Saito[1], Tatjana Thomas[1], Yassine Agarmani[1], Tim Thyzel[1], Kenichiro Hashimoto[2], Takahiko Sasaki[2,3], Jens Müller[1], and Michael Lang[1] — [1]Goethe University Frankfurt, Frankfurt (M), Germany — [2]University of Tokyo, Chiba, Japan — [3]Tohoku University, Sendai, Japan

Geometrical frustration causes degenerate states and a frustrated charge system is proposed in organic conductors. It is expected that charge order (CO) is suppressed and is possibly replaced by a charge glass state. In organic condutors, the CO transition accompanies a structural transition. Therefore, investigating their elastic properties is of fundamental interest. We performed thermal expansion measurements on θ-$(BEDT\text{-}TTF)_2MM'(SCN)_4$ (MM' = CsZn, CsCo, and RbZn) : whereas the CsZn and CsCo salts exhibit no CO transition, slowly-cooled RbZn salt shows the transition. The thermal expansion coefficient of no-CO salts exhibited a glassy transition at 90-100 K. This behavior is reminiscent of the freezing of the terminal ethylene end-groups on the BEDT-TTF molecules. For the RbZn salt we observe a CO transition at 210 K and also an ethylene-group related glass-like transition at 80-100 K. Therefore, the glass-like anomaly around 90 K appears as a common feature in θ-type salts regardless of whether long-range CO exists. These results point to the importance of the lattice degrees of freedom in the frustrated charge system.