TT 42: Charge Order

Time: Tuesday 10:15–13:00 Location: HFT-FT 131

TT 42.1 Tue 10:15 HFT-FT 131

Charge order and Frustration on the triangular lattice - A Monte Carlo Study of the Falicov-Kimball model — •Miguel M. Oliveira[1], Andrey Antipov[3], Pedro Ribeiro[1], and Stefan Kirchner[2] — [1]Instituto Superior Técnico, Universidade de Lisboa Av. Rovisco Pais, 1049-001 Lisboa, Portugal — [2]Center for Correlated Matter, Zhejiang University, Hangzhou, Zhejiang 310058, China — [3]Station Q, Microsoft Research, Santa Barbara, California 93106, USA

The Falicov-Kimball model is commonly used as one of the simplest possible models to study the metal-insulator transition. Recently, it has been shown that the half-filled Falicov-Kimball model on the square lattice, above the charge order transition, has a richer phase diagram than originally anticipated [1].

In this talk we present the extension of these results to the triangular lattice. In particular, for 1/3 filling, we find that the high temperature disordered phases are similar to those found for the half-filled square lattice.

At low temperatures and large coupling, the ordered phase has a broken Z_3 symmetry and the transition into this state is of the same universality as the three-state Potts model.

We investigate the possibility that frustration effects in the weak-coupling regime and at low temperatures may destroy the Z_3-broken phase and induce other kinds of ordered or liquid states.

[1] A.Antipov et al PRL **117** 146601 (2016).

TT 42.2 Tue 10:30 HFT-FT 131

Density Matrix Renormalization Group Study of the Two-Dimensional Hubbard Model in Hybrid Real-Momentum Space — •Georg Ehlers and Reinhard M. Noack — Philipps Universität Marburg

We investigate the square-lattice Hubbard model in hybrid real-momentum space using the density matrix renormalization group (DMRG). The variation of the DMRG that we use is formulated for lattices with cylindrical geometry and utilizes the conserved transverse lattice momentum. Compared to the standard real-space algorithm, it achieves a speedup that scales quadratically with the width of the lattice [G. Ehlers et al., Phys. Rev. B 95, 125125 (2017)]. For width-four and width-six cylinders at one-eighth doping and Coulomb interaction strengths U/t=8 and U/t=4, we find a striped ground state. In a combined study with other state-of-the-art numerical methods, we provide strong evidence that the striped state is present in a substantial region of the underdoped regime of the ground-state phase diagram of the two-dimensional Hubbard model. The periodicity and stripe filling of our striped state differs from that found experimentally in hole-doped cuprates, indicating that terms beyond the standard Hubbard model must be included to accurately model high-temperature superconductivity [1].

[1] B.-X. Zheng et al., Science 358, 1155 (2017).

TT 42.3 Tue 10:45 HFT-FT 131

Dynamical manipulation of crystalline symmetry — Tanay Nag, R-J Slager, and •Takashi Oka — Max Planck Institute for Physics of Complex Systems (MPI-PKS), Dresden, Germany

Our main aim is to break a discrete symmetry of honeycomb lattice model by introducing suitable laser field. Unlike the laser field with single frequency that is not able to generate a inversion symmetry breaking on-site momentum independent mass term, a bi-harmonic laser filed with commensurate frequencies can break the C_3 symmetry of the model and lead to a finite charge density wave order. We show that there is a possibility that the CDW shows memory effect (hysteresis). In order to enhance the CDW order, we consider an extended Hubbard interaction implemented through a mean field approach. We explain the synchronization dynamics of CDW in the switch on and switch off region by making resort to a simple toy model namely, Kuramoto model. Furthermore, we show that van Hove singularity in density of states for this model substantially contributes to the dynamics.

TT 42.4 Tue 11:00 HFT-FT 131

Supercooled and hidden electronic phases in thin 1T-TaS_2 — •Quirin Stahl[1], Tobias Ritschel[1,2], Maximilian Kusch[1], Florian Heinsch[1,3], Gaston Garbarino[4], Norman Kretzschmar[4], and Jochen Geck[1] — [1]TU Dresden, Germany — [2]UBC, Vancouver, Canada — [3]HZDR, Germany — [4]ESRF, Grenoble, France

The ultra-fast semiconductor-to-metal transition in nano-thick 1T-TaS_2 crystals induced by femtosecond laser pulses currently attracts a lot of interest [1,2]. In particular, since it is believed that such laser pulses stabilize so-called hidden states, which cannot be reached from thermal equilibrium and which exhibit unique electronic properties. We present a detailed XRD study of nano-thick 1T-TaS_2 single crystals. In a first experiment we studied the charge density wave order in the supercooled state, which has been observed earlier in resistivity measurements[3]. This phase is then compared to the charge density wave order created by a femto-second laser pulse. We find that the supercooled and the hidden electronic phases are identical within the error of the experiment, implying that the hidden state of 1T-TaS_2 is a supercooled NC-CDW state. These results will be discussed in terms of unusual phase ordering kinetics caused by a down-scaling of the sample thickness into the nanometer-regime.

[1] L. Stojchevska *et al.*, Science 334, 177 (2014)
[2] I. Vaskivskyi *et al.*, Science Advances 1, 6 (2015)
[3] M. Yoshida *et al.*, Scientific Reports 4, 7302 (2014)

TT 42.5 Tue 11:15 HFT-FT 131

Temperature-dependence of the three-dimensional band structure of 1*T*-TaS_2 — •Sanjoy K. Mahatha[1], Arlette S. Ngankeu[1], Kevin Guilloy[1], Marco Bianchi[1], Charlotte E. Sanders[1], Kerstin Hanff[2], Kai Rossnagel[2], Jill A. Miwa[1], Christina Breth Nielsen[3], Martin Bremholm[3], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, 8000 Aarhus C, Denmark — [2]Institute for Experimental and Applied Physics, Kiel University, Germany — [3]Department of Chemistry, University of Aarhus, Aarhus, Denmark

The 1*T* polymorph of the layered transition metal dichalcogenide compound TaS_2 undergoes a series of temperature-dependent phase transitions consisting of periodic structural distortions and organization of the electrons into regular patterns known as charge density waves (CDW). The different CDW phases vary remarkably in their electronic properties. The commensurate CDW phase of 1*T*-TaS_2 has widely been studied as a quasi-two-dimensional phenomenon that coexists with a Mott insulating state. However, recent theoretical calculations predicted the coexistence of the CDW phase with a nearly one-dimensional metallic dispersion perpendicular to the crystal planes. Our recent angle-resolved photoemission spectroscopy results confirm the existence of a dispersive band which exists for all the different CDW phases at different temperatures. Here, we will give a detailed account of the three dimensional band structure of this highly correlated material.

TT 42.6 Tue 11:30 HFT-FT 131

Zigzag-chain domain walls facilitate metalisation of the Mott insulator on a triangular lattice — Jan Skolimowski[1] and •Rok Žitko[1,2] — [1]Jožef Stefan Institute, Jamova 39, Ljubljana, Slovenia — [2]Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 19, Ljubljana, Slovenia

Motivated by the occurrence of a long-lived metastable metallic hidden-state in 1T-TaS_2 that can be induced by optical or voltage pulses and that shows a characteristic mosaic pattern of mesoscale charge-density-wave (CDW) domains separated by a dense web of domain walls, we study how the structural domain walls affect the electron dynamics. We consider the Hubbard model on a triangular lattice as a low-energy effective model describing the narrow electron band formed around the Fermi level in the low-temperature commensurate $\sqrt{13} \times \sqrt{13}$ phase of 1T-TaS_2. Within the effective model a domain wall between two CDW domains leads to a local modification of the hopping constants along a one-dimensional defect line. We study the resulting Hamiltonian using the extension of the dynamical mean-field theory to inhomogeneous systems. We discuss in detail the case where the hopping constants are enhanced and the domain wall metallises. We show that this is facilitated by the fact that in the triangular lattice the domain walls tend to enhance the hopping constants along a connected zigzag line, rather than forming a ladder of dimers which instead show a band gap. We also discuss the case of multiple domain walls and comment on the relevance of the domain-wall-metallisation scenario for the metallic hidden-state.

15 min. break.

TT 42.7 Tue 12:00 HFT-FT 131

Competition of strong charge and spin fluctuations in monolayer NbS_2 — •Erik van Loon[1], Malte Rösner[2,3], Gunnar Schönhoff[3], Mikhail Katsnelson[1], and Tim Wehling[3] — [1]Radboud Universiteit, Nijmegen, Nederland — [2]University of Southern California, Los Angeles, USA — [3]Universität Bremen, Bremen, Deutschland

Single-layers of transition metal dichalcogenides have rich phase diagrams featuring metallic, insulating and charge/spin density wave phases. Competing interactions lie beneath these competing phases. Theoretical descriptions have so far focussed on the electron-phonon interactions in these materials, whereas the electron-electron interaction has mostly been ignored. In this talk, we show that in NbS_2 the local Coulomb interaction is by itself strong enough to turn the material insulating. Screening by the electron-phonon and the non-local Coulomb interaction restores the metallic phase, leads to a broadening of the electronic spectral function and to a coexistence of strong charge and spin fluctuations. These results are obtained by combining an abinitio determination of the band structure and Coulomb interaction with the Dual Boson approach for the extended Hubbard model.

TT 42.8 Tue 12:15 HFT-FT 131

Three-Dimensional Fermi Surface of $2H$-$NbSe_2$ - Implications for the Mechanism of Charge Density Waves — •Roland Hott[1], Frank Weber[1], Rolf Heid[1], Leonid L. Lev[2], Thorsten Schmitt[2], and Vladimir N. Strocov[2] — [1]Institute for Solid State Physics, Karlsruhe Institute of Technology, D-76021 Karlsruhe, Germany — [2]Paul Scherrer Institut, Swiss Light Source, CH-5232 Villigen PSI, Switzerland

We investigated the three-dimensional electronic structure of the seminal charge-density-wave (CDW) material $2H$-$NbSe_2$ by soft x-ray angle-resolved photoelectron spectroscopy and density-functional theory. Our results reveal the pronounced 3D character of the electronic structure formed in the quasi-two-dimensional layered crystal structure. In particular, we find a strong dispersion along k_z excluding a nesting-driven CDW formation based on experimental data.

TT 42.9 Tue 12:30 HFT-FT 131

The Coherent Response in the Ground State of the Excitonic Insulator Ta_2NiSe_5 — •Minjae Kim[1,2], Parmida Shabestari[1,2], Emily Huang[1,2], Daniel Werdehausen[1,2], Steinn Ymir Agustsson[1,2], Timofei Larkin[1], Alexander Boris[1], Tomohiro Takayama[1,2], Hao Chu[1,2], Hidenori Takagi[1,2], and Stefan Kaiser[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]University of Stuttgart, Germany

The excitonic insulator (EI) is an intriguing phase of condensed excitons undergoing a BEC-type transition. A prominent candidate has been identified in Ta_2NiSe_5 [1]. Ultrafast spectroscopy allows tracing the coherent response of the EI condensate directly in the time domain. Probing the collective electronic response we can identify the Higgs-amplitude mode of the condensate. In addition we find a peculiar coupling of the EI phase to a low frequency phonon mode [2]. We will discuss the transient response on multiple energies scales ranging from the exciton dynamics in the NIR down to the coherent THz response of the gap.

[1] Y.F. Lu et al., Nat. Comm. 8, 14408 (2017).
[2] D. Werdehausen et al., arXiv:1611.01053 (2016).

TT 42.10 Tue 12:45 HFT-FT 131

Nearfield Optical Probe of the Excitonic Insulator Transition in Ta_2NiSe_5 — •Amrit Raj Pokharel[1,2], Heiko Linnenbank[2], Tomohiro Takayama[1,2], Hidenori Takagi[1,2], and Stefan Kaiser[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]University of Stuttgart

The Excitonic Insulator (EI) is an intriguing phase of condensed excitons that undergo Bose Einstein Condensation (BEC). A prominent solid-state candidate for an EI is Ta_2NiSe_5, which is a quasi-onedimensional material that undergoes a semiconductor to excitonic insulator phase transition at T_c=328K [1]. Here we investigate the formation of the excitonic gap using Scattering-Scanning Nearfield Optical Microscope (s-SNOM). That allows us tracing the optical response with spatial resolution down to tens of nanometer when the system is driven across T_c by temperature. Probing at different energy scales - in the gap, at the exciton peaks and close to strongly coupled phonons - reveals the nature of the EI transition. We will discuss a homogeneous gap and an inhomogeneous near field pattern on the exciton peak around T_c with respect to the second order nature of the phase transition.

[1] Y.F.Lu, et al. Nat.Com. 8, 14408 (2017).