HL 31: Focus Session: Frontiers of Electronic-Structure Theory V (joint session O/HL)

Time: Wednesday 15:00–17:30 Location: TRE Ma

HL 31.1 Wed 15:00 TRE Ma

Phase transitions in the two-dimensional Su-Schrieffer-Heeger model — •Changan Li[1], Songbo Zhang[2], Sangjun Choi[1], Jan Budich[3], and Björn Trauzettel[1] — [1]Institute for theoretical physics and astrophysics, University of Würzburg, Wuerzburg, Germany — [2]Department of Physics, University of Zürich, Winterthurerstrasse 190 8057, Zürich, Switzerland — [3]Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany

The 2D Su-Schrieffer-Heeger (SSH) model is endowed with rich topological physics. First we show that the random flux can induce a metal-band insulator transition in the 2D SSH, thus reporting the first example of such a transition. Remarkably, we find that the resulting insulating phase can even be a higher-order topological insulator with zero-energy corner modes and fractional corner charges. Employing both level statistics and finite-size scaling analysis, we characterize the metal-band insulator transition and numerically extract its critical exponent. By proposing another inclined 2D SSH model, a deformed one, we show that a pair of Dirac points protected by space-time inversion symmetry appear in the semimetallic phase. Interestingly, the locations of these Dirac points are not pinned to any high-symmetry points of the Brillouin zone but highly tunable through parameter modulations. Moreover, the merging of two Dirac points undergoes a topological phase transition, which leads to either an anisotropic topological insulating phase or a nodal-line metallic phase.

HL 31.2 Wed 15:15 TRE Ma

Ab initio embedding approach for carbon defects in hexagonal boron nitride: A new platform to probe environmental screening — •Danis Badrtdinov[1], Magdalena Grzeszczyk[2], Alexander Hampel[3], Cyrus Dreyer[3,4], Maciej Koperski[2], and Malte Rösner[1] — [1]Radboud University, Nijmegen, The Netherlands — [2]National University of Singapore, Singapore — [3]Flatiron Institute, USA — [4]Stony Brook University, USA

Correlated defects in layered van der Waals hosts hold high promises for realizing quantum technologies, as they allow for various possibilities to control defect properties, e.g., via altering the host thickness or by changing the substrate material. A quantitative description of the defect ground and excited states taking the details of the impurity environment into account is, however, a considerable challenge for conventional density-functional theory (DFT) based methods as the impurities might be correlated and dielectric environmental screening is not fully accounted for in DFT. To tackle these challenges we apply and extend an embedding approach that treat the defect states within exact many-body theory, while DFT is used as a starting point to describe the bulk host material. We study various carbon defects embedded in hexagonal boron nitride (hBN), allowing us to disentangle all mechanisms responsible for the alteration of defect properties including modifications to the impurity structure and changes in the environmental screening upon thinning down the hBN host. Our new embedding approach paves the way for improved identification of defects in layered materials and to tailor their properties.

HL 31.3 Wed 15:30 TRE Ma

Nonequilibrium electron dynamics in a two-sites Hubbard model — •Jakub Wronowicz and Yaroslav Pavlyukh — Department of Theoretical Physics, Wrocław University of Science and Technology

Electron dynamics in a two-sites Hubbard model is studied using the nonequilibrium Green's function approach using formalism developed in [1]. We focus on the electron dynamics arising in the adiabatic switching scenario. Many-body approximations are classified according to the channel of the Bethe-Salpeter equation in which electronic correlations are explicitly treated. They give rise to the so-called second Born, T-matrix and GW approximations. In each of these cases, the model is reduced to a system of ordinary differential equations, which resemble equations of motion for a driven harmonic oscillator with time-dependent frequencies. We discuss transient solutions for the off-diagonal density matrix. Analytical result for the steady state in second Born approximation is compared with the exact solution. It is further shown numerically that in the large Hubbard-U limit the T -matrix in the particle-hole channel and spin-adapted GW approximations converge to the same solution.

[1] Y. Pavlyukh, E. Perfetto, and G. Stefanucci, *Photoinduced dynamics of organic molecules using nonequilibrium Green's functions with second-Born, GW, T-matrix, and three-particle correlations*, Phys. Rev. B **104**, 035124 (2021).

HL 31.4 Wed 15:45 TRE Ma

Time-linear quantum transport simulations with correlated nonequilibrium Green's functions — •Riku Tuovinen[1], Yaroslav Pavlyukh[2], Enrico Perfetto[3], and Gianluca Stefanucci[3] — [1]Department of Physics, Nanoscience Center, University of Jyväskylä, Finland — [2]Department of Theoretical Physics, Wroclaw University of Science and Technology, Poland — [3]Dipartimento di Fisica, Università di Roma Tor Vergata, Italy

We present a time-linear scaling method for open and correlated quantum systems. The method inherits from many-body theory [1] the possibility of selecting the most relevant scattering processes, thereby paving the way for real-time characterizations of correlated ultrafast phenomena in quantum transport. The open system dynamics is described in terms of an embedding correlator from which the transient current can be calculated via the Meir-Wingreen formula [2]. We efficiently implement the method through a combination with recent time-linear schemes for closed systems [3]. Electron-electron and electron-phonon interactions can be treated on equal footing while preserving all fundametal conservation laws. We employ the method by studying transport of correlated electron-hole pairs in semiconductors [4].

[1] G. Stefanucci and R. van Leeuwen, Nonequilibrium Many-Body Theory of Quantum Systems (CUP 2013).

[2] Y. Meir and N. S. Wingreen, PRL 68, 2512 (1992).

[3] N. Schlünzen, J.-P. Joost, and M. Bonitz, PRL 124 (2020) 076601.

[4] R. Tuovinen, Y. Pavlyukh, E. Perfetto, and G. Stefanucci, arXiv:2211.15635 (2022).

15 min. break

Topical Talk HL 31.5 Wed 16:15 TRE Ma

Challenges in modelling correlated electronic matter — •Roser Valenti — Institute of Theoretical Physics, Goethe University Frankfurt, Frankfurt, Germany

The microscopic modelling of correlated electronic matter from first principles poses a fundamental theoretical challenge due to the many-body character of the systems. In recent years there have been a few internationally coordinated efforts in theoretical method development to generate a common platform of benchmarked software tools including dynamical mean field theory and extensions.

In this talk I will present some of the challenges we face in such an endeavour and illustrate them with some examples on models and materials.

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HL 31.6 Wed 16:45 TRE Ma

Electron-Phonon Interactions from DFPT within an All-Electron Framework — •Sebastian Tillack, Pasquale Pavone, and Claudia Draxl — Humboldt-Universität zu Berlin and IRIS Adlershof, 12489 Berlin, Germany

The interplay between electrons and the motions of nuclei in solids, described in terms of phonons, play a crucial role in the modeling of functional materials, particularly for understanding temperature dependent effects. We present an implementation of density-functional perturbation theory (DFPT) within a full-potential all-electron framework as implemented in the code `exciting` [1]. Our implementation allows one to compute phonons as well as the linear response to external electric fields. We use DFPT calculations to study lattice vibrations and electron-phonon interactions (EPIs) by means of many-body perturbation theory in β-Ga_2O_3. The electron self-energy contribution is computed as a function of temperature from which various properties such as quasi-particle energies, electron linewidths, and spectral functions are derived. We further incorporate many-body electron-electron interactions described by the GW method. Beyond that, our work creates the foundation for a fully *ab initio* study of the effect of EPIs on

optical excitations.

[1] A. Gulans, et al. J. Phys.: Condens. Matter 26, 363202 (2014).

HL 31.7 Wed 17:00 TRE Ma

Calculation of phonon spectra with the FLAPW method using Density Function Perturbation Theory — •Alexander Neukirchen, Christian-Roman Gerhorst, Gregor Michalicek, Daniel Wortmann, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Computing phonons applying density functional perturbation theory (DFPT) within all-electron DFT methods is a well-known challenge due to the displacement of muffin-tin spheres and sphere-centered basis functions. In this talk, we present our current results of the phonon dispersion based on our implementation of the DFPT approach in the FLEUR code [1] (www.flapw.de), an implementation of the full-potential linearized augmented plane wave (FLAPW) method. We highlight the good agreement of our preliminary results with phonon dispersions obtained with the finite displacement method for which the FLEUR code has been combined with the phonopy tool (www.phonopy.github.io/phonopy/). We discuss the numerical challenges involved in calculating meV quantites on top of large ground state energies typical for all-electron methods and how we addressed them.

This work has been supported by the Helmholtz Postdoc Programme (VHPD-022) and by the MaX Center of Excellence funded by the EU through the H2020-INFRAEDI-2018-1 767 (Grant No. 824143).

[1] A. Neukirchen, C.-R. Gerhorst, D. A. Klüppelberg, M. Betzinger, D. Wortmann, G. Michalicek, G. Bihlmayer, S. Blügel, to be published.

HL 31.8 Wed 17:15 TRE Ma

Electron-phonon interaction using a localized Gaussian basis set — •Gerrit Johannes Mann, Thorsten Deilmann, and Michael Rohlfing — Institute of Solid State Theory, University of Münster, Germany

Electron-phonon interaction is a crucial mechanism in solid state physics that is responsible for a multitude of phenomena. However, in electronic structure calculations it is usually neglected. We developed an ab-initio implementation on top of density functional theory that combines finite differences calculations with the perturbative Allen-Heine-Cardona framework in order to calculate the temperature-dependent renormalization of the electronic bandstructure due to electron-phonon interaction using a basis set of localized Gaussian orbitals.

This implementation circumvents the limiting problems of previous implementations while maintaining a good agreement with the literature. The calculated Fan-Migdal zero-point renormalization of the direct band gap of silicon amounts to about 15 meV compared to 20 meV in the literature. Also the temperature-dependence of the renormalization agrees similarly well.