SYES 1: Advances in Ab-Initio Electronic Structure Theory of Time-Dependent and Non-Equilibrium Phenomena

Time: Tuesday 9:30–12:15 Location: H 0105

Invited Talk SYES 1.1 Tue 9:30 H 0105

Light control of charge transport and phase transitions — •Sheng Meng — Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

Photoexcitation is a powerful means in distinguishing different interactions and manipulating the properties of matter, especially for charge transport and phase transitions in complex quantum systems. Here we show that laser-controlled coherent phonon excitation enables orders of magnitude enhancement of carrier mobility via accelerating polaron transport in a prototypical material, lithium peroxide. The selective excitation of specific phonon modes, whose vibrational pattern directly overlap with the polaronic lattice deformation, can remarkably reduce the energy barrier for polaron hopping. The strong nonadiabatic couplings between the electronic and ionic subsystem play a key role in triggering charge transport. These results extend our understanding of charge transport dynamics to the nonequilibrium regime and allow for optoelectronic devices with ultrahigh on-off ratio and ultrafast responsibility competitive with those of state-of-the-art devices. We also investigate photoexcitation induced ultrafast phase-transition dynamics in two-dimensional materials, where we identify a laser-induced collective pathway from 2H phase to 1T phase in MoTe2 that is significantly different from thermal phase transitions. Our results provide insights from a new perspective on the coherent electron and lattice quantum dynamics in materials upon photoexcitation.

Invited Talk SYES 1.2 Tue 10:00 H 0105

Probing the transport of the interacting electron-phonon system self-consistently and *ab initio* — •Nakib Protik — Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Germany

In the materials where phonons and the charge carriers coexist and interact with each other, the transport of one system induces the transport of the other. This is known as the mutual electron-phonon drag. In order to capture the dragful charge, heat, and thermoelectric transport in such materials, the kinetic equations of both types of quasiparticles have to be solved self-consistently. While the formal structure of the coupled kinetic equations has been known since 1930 [1], it is only recently that a fully *ab initio*, coupled electron-phonon Boltzmann transport formalism, called `elphbolt` [2], has been developed. This has opened the avenue for the parameters-free and *in silico* probing of the dragful transport. In this talk, I will outline the theoretical and computational underpinnings of the `elphbolt` framework and how it can be used for predicting and explaining the various transport phenomena in materials. I will discuss some of the new developments in the project along with possible future research directions.

[1] Peierls, R. Zur Theorie der elektrischen und thermischen Leitfähigkeit von Metallen. Ann. Phys. 396, 121-148 (1930).

[2] Protik, N.H., Li, C., Pruneda, M. et al. The elphbolt ab initio solver for the coupled electron-phonon Boltzmann transport equations. npj Comput Mater 8, 28 (2022).

Invited Talk SYES 1.3 Tue 10:30 H 0105

In- and out-of-equilibrium ab initio theory of electrons and phonons — •Gianluca Stefanucci — Universita di Roma Tor Vergata, Italy

We lay down the ab initio many-body quantum theory of electrons and phonons in equilibrium as well as in steady-state or time-varying settings [1]. The focus is on the harmonic approximation, but the developed tools can readily incorporate anharmonic effects. We begin by showing the necessity of determining the ab initio Hamiltonian in a self-consistent manner to ensure the existence of an equilibrium state. We then identify the correct partitioning into a noninteracting and an interacting part to carry out diagrammatic expansions in terms of dressed propagators and screened interactions. The final outcome is the finite-temperature nonequilibrium extension of the Hedin equations, showcasing the emergence of the coupling between electrons and coherent phonons through the time-local Ehrenfest diagram. We also derive the Kadanoff-Baym equations, discuss the theory of conserving approximations, and highlight the simplifications leading to the Born-Oppenheimer approximation as well as the semiconductor Bloch and Boltzmann equations.

[1] G. Stefanucci, R. van Leeuwen and E. Perfetto, Phys. Rev. X 13, 031026 (2023)

15 min. break

Invited Talk SYES 1.4 Tue 11:15 H 0105

Phonon screening of excitons in semiconductors and insulators from first principles — •Marina Rucsandra Filip — University of Oxford, Department of Physics

Excitons are correlated electron hole pairs, which form in semiconductors and insulators upon absorption of light. Understanding the formation, dynamics and dissociation of excitons is of key importance for optoelectronic applications, such as photovoltaic and light emitting devices. First principles methods based on the GW + Bethe Salpeter equation (BSE) [1] have been playing a key role in developing this understanding from an atomistic perspective. In this talk, I will discuss a framework that we have recently developed [2,3], to understand the role played by ionic vibrations on the properties of excitons. I will motivate this development by highlighting the importance of phonons for the dielectric screening of excitons using a model Wannier-Mott (hydrogenic) picture, and parameters corresponding to well known semiconductors (III-V, halide perovskites). I will then show how this model picture can be generalized into a first principles approach, based on the standard GW+BSE framework. I will show how our implementation allows us to perform fully converged calculations of phonon screening effects, and identify the carrier-phonon interactions which dominate phonon screening in different materials. [1] Rohlfing & Louie, Phys. Rev. Lett. 81, 2312 (1998). [2] Filip, Haber & Neaton, Phys. Rev. Lett., 127, 067401 (2021). [3] Alvertis, Haber, Li, Coveney, Louie, Filip & Neaton, Submitted (2023). Work supported by the EPSRC, with computational resources from TACC at UT Austin.

Invited Talk SYES 1.5 Tue 11:45 H 0105

Light-matter control of quantum materials: from Floquet to cavity engineering — •Michael Sentef — Institute for Theoretical Physics and Bremen Center for Computational Materials Science, University of Bremen, 28359 Bremen, Germany — Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany

Advances in time-resolved pump-probe spectroscopies have enabled us to follow the microscopic dynamics of quantum materials on femtosecond time scales. This gives us a glimpse into the inner workings of how complex, emergent functionalities of quantum many-body systems develop on ultrafast time scales or react to external forces. The ultimate dream of the community is to use light as a tuning parameter to create new states of matter on demand with designed properties and new functionalities, perhaps not achievable by other means. In this talk I will discuss recent progress in controlling and engineering properties of quantum materials through light-matter interaction. I will highlight work on Floquet engineering – the creation of effective Hamiltonians by time-periodic drives – on sub-cycle time scales combining theory and pump-probe experiments at the limits of energy and time resolution. I will then showcase recent theories on inducing superconductivity with light by employing enhanced light-matter interaction in the near-field involving polaritonic excitations.