# O 58: Focus Session: Electron-Phonon Interactions II

Time: Wednesday 15:00–17:15 Location: H15

**Invited Talk** O 58.1 Wed 15:00 H15

**Towards a systematic way of treating non-adiabatic effects** — •E.K.U. Gross — Max Planck Institut of Microstructure Physics, 06120 Halle, Germany

Some of the most fascinating quantum phenomena, such as the process of vision or phonon-driven superconductivity are examples of non-adiabatic effects. To treat such phenomena in a genuine first-principles way, one has to start from the full Hamiltonian of the complete system of electrons and nuclei. We employ the exact factorization [Abedi, Maitra, Gross, PRL 105, 123002 (2010)] of the full electron-nuclear wavefunction into a purely nuclear part and a many-electron wavefunction which parametrically depends on the nuclear configuration and carries the meaning of a conditional probability amplitude. The equations of motion of these wavefunctions uniquely define "exact phonons" beyond the Born-Oppenheimer approximation and the electron-phonon interaction (to all orders) in a very compact way. In addition to the exact potential energy surface there appears a Berry-type vector potential in the ionic equation of motion which gives rise to a geometric phase beyond the Born-Oppenheimer limit. We discuss how this exact geometric phase differs from the Born-Oppenheimer Berry phase, and how this difference can potentially be measured [Requist, Proetto, Gross, PRA 96, (6), 062503, (2017)]. In the time-domain, we deduce, from the exact equations of motion, a novel mixed-quantum-classical algorithm [Min, Agostini, Tavernelli, Gross, JPCL 8, 3048 (2017)] which provides a much improved (over surface hopping) description of decoherence.

O 58.2 Wed 15:30 H15

**Exact factorization density functional theory of electron-phonon systems** — •Ryan Requist[1], Cesar Proetto[2], and Eberhard K. U. Gross[1,3] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Centro Atomico Bariloche and Instituto Balseiro, San Carlos de Bariloche, Argentina — [3]Fritz Haber Center for Molecular Dynamics, Jerusalem, Israel

In this talk, I will discuss how to generalize density functional theory to incorporate nonadiabatic electron-phonon coupling effects. Kohn-Sham equations that yield the electronic density $n_U(\mathbf{r})$, conditional on the set of all phonon normal mode amplitudes $U = \{U_{\mathbf{q}\lambda}\}$, are coupled to the nuclear Schrödinger equation of the exact factorization scheme [1,2]. An orbital-dependent functional approximation for the nonadiabatic exchange-correlation energy is proposed. It is shown to exactly reproduce the leading-order nonadiabatic electron-phonon coupling effects, e.g. electronic velocity renormalization, in the Fröhlich model.

[1] Phil. Trans. Roy. Soc. A 372, 20130059 (2014); [2] Phys. Rev. Lett. 105, 123002 (2010)

O 58.3 Wed 15:45 H15

**Superconductivity from first-principles in sodalite yttrium hydrides** — •Simone Di Cataldo[1], Christoph Heil[1], Lilia Boeri[2], and Giovanni Bachelet[2] — [1]Institute of Theoretical and Computational Physics, Graz University of Technology, NAWI Graz, 8010 Graz, Austria — [2]Dipartimento di Fisica, Sapienza Università di Roma, 00185 Roma, Italy

The recent experimental discovery of the record-breaking critical superconducting temperature of 265 K in a lanthanum superhydride ($LaH_{10}$ ), following the one of 203 K in $SH_3$ three years ago, firmly supports hydrides as promising candidates in the search for room-temperature superconductivity.

In our work we use Density Functional Theory, together with fully anisotropic first-principles Migdal-Eliashberg theory to investigate the electronic, vibrational and superconducting properties of two yttrium hydrides ($YH_6$ and $YH_{10}$), which are closely related to the corresponding lanthanum hydrides, but have been predicted to exhibit even higher $T_c$s. We show that the superconducting properties are rather uniform over all phonon and electronic states, meaning that the origin of the strong electron-phonon coupling cannot be explained only in terms of the hydrogen sublattice, but is rather due to the interaction between the host atom and the whole clathrate sublattice. A comparison of the pressure behavior of the $T_c$ of the two compounds suggests a route to lower the pressure to high $T_c$ superconductivity.

O 58.4 Wed 16:00 H15

**No superconductivity in iron polyhydrides at high pressures** — •Lilia Boeri[1], Christoph Heil[2], and Giovanni Bachelet[1] — [1]Dipartimento di Fisica, Sapienza Universita' di Roma, Italy — [2]ITP-CP, Graz University of Technology, Austria

A recent experimental study [1] reported the formation of several new iron polyhydrides FeHx at pressures in the megabar range and spotted FeH5, which forms above 130 GPa, as a potential high-Tc superconductor because of an alleged layer of dense metallic hydrogen. Shortly after, two studies based on ab initio Migdal-Eliashberg theory seemed to independently confirm such a conjecture. We conversely find, on the same theoretical-numerical basis, that neither FeH5 nor its precursor, FeH3, shows any conventional superconductivity and explain why this is the case.

[1] C. Pepin et al., Science 357, 382 (2017).

O 58.5 Wed 16:15 H15

**Simulation of electronic friction effects in chemical dynamics at metal surfaces: Understanding the successes and failures of ab-initio methods** — •Connor Box and Reinhard J. Maurer — Department of Chemistry, University of Warwick, United Kingdom

The coupling of molecular adsorbate motion with hot electrons in a metal substrate represents a breakdown of the Born-Oppenheimer approximation with measurable consequences. An accurate theoretical description of how these hot electron effects modify the reaction dynamics of molecules on metals will be essential to utilize light-matter interaction in catalysis. The electron-phonon coupling between adsorbate vibrations and hot electrons are efficiently described in a density functional theory-based molecular dynamics with electronic friction (MDEF) approach, where electronic friction forces act on atoms within a Langevin framework. [1] Several methods have been proposed to describe electronic friction; however, more work remains to be done to provide a transferable and accurate description of experimental findings. In this talk, we present our efforts towards pushing beyond the current limitations of the MDEF method. We explore the consequences of existing approximations in MDEF calculations for the frequently studied carbon monoxide adsorbed Cu(100) and Pt(111) surfaces. [2] We systematically assess the importance of substrate motion, vibrational anharmonicity, and mode coupling in comparison with recently published many-body perturbation theory results [3] to guide future directions of method development. [1] PRL 116, 217601 (2016), [2] PRB 94, 115432 (2016), [3] PRL 120, 156804 (2018)

O 58.6 Wed 16:30 H15

**Nonadiabatic effects in electron and phonon spectra of electron-doped monolayer $MoS_2$ from first-principles calculations** — •peio garcia-goiricelaya[1,2], jon lafuente-bartolome[1,2], idoia g.gurtubay[1,2], and asier eiguren[1,2] — [1]Materia Kondentsatuaren Fisika Saila, University of the Basque Country UPV/EHU, 48080 Bilbao, Basque Country, Spain — [2]Donostia Interational Physics Center (DIPC), Paseo Manuel de Lardizabal 4, 20018 Donostia-San Sebastián, Spain

We present a complete *ab initio* analysis of the electron-phonon interaction in the electron-doped monolayer $MoS_2$, a system that is attracting growing interest, specially after the discovery of gate-induced spin-locking superconductivity [1]. Also recently, intriguing renormalized band structure has been observed in this system [2], which calls into question the exact mechanism by which electron-phonon interaction is so effective. Our calculations uncover the exceptional quasiparticle band-splitting structure. Directly connected to the renormalized electron structure, we complement the study by analyzing the nonadiabatic phonon spectrum, where we predict also strong vibrational branch renormalization for some modes. These results are illustrated with the help of simplified model calculations.

[1] Ye, J.T. *et al.* Superconducting dome in a gate-tuned band insulator. *Science* **338**, 1193-1196 (2012).

[2] Kang, M. *et al.* Holstein polaron in a valley-degenerate two-dimensional semiconductor. *Nature Materials* **17**, 676-680 (2018).

O 58.7 Wed 16:45 H15

**Phonon renormalization in ab-initio-based lattice models** — •Jan Berges[1], Malte Roesner[2,3], Erik van Loon[1], and Tim

Wehling[1] — [1]Institute for Theoretical Physics and Bremen Center for Computational Materials Science, University of Bremen, Germany — [2]Department of Physics and Astronomy, University of Southern California, Los Angeles, USA — [3]Center for Computational Quantum Physics, Flatiron Institute, New York, USA

Phonons play a major role in the understanding of phenomena such as superconductivity, periodic lattice distortions, magnetostriction, thermo- and piezoelectrics. Yet, despite the success of *density-functional perturbation theory* (DFPT), their ab-initio calculation remains challenging for structurally complex and strongly interacting systems. To address these problems, we introduce a computational scheme based on material-realistic quantum lattice models, that combine the efficiency of a lattice model with an ab-initio input and the freedom to choose different levels of approximation to treat electron-electron interactions. In our scheme, all parameters are derived ab initio, using the *constrained* methods cRPA and cDFPT [Nomura, Arita: Phys. Rev. B **92**, 245108 (2015)]. In the presented work, we apply our scheme to the metallic *transition-metal dichalcogenides* (TMDCs), prominent showplace for coexisting many-body instabilities. First, we demonstrate that the fully renormalized ab-initio results are exactly reproduced by our model if we solve it at the level of the *random-phase approximation* (RPA). Then we study the influence of charge doping and hybridization with substrates.

O 58.8 Wed 17:00 H15

**Efficient calculation electron-phonon related problems thought Helmholtz Fermi Surface harmonics (HFSH).** — Jon Lafuente-Bartolome[1,2], Idoia G. Gurtubay[1,2], and •Asier Eiguren[1,2] — [1]Condensed Matter Physics Dept. Uni. Basque Country (UPV/EHU), Spain — [2]Donostia International Physics Center (DIPC), San Sebastian, Spain

In a metals, the details ls of the Fermi surface and the magnitude of the matrix elements connecting different points defined on it determine most of the transport properties, which are limited by the electron-phonon coupling and the scattering by impurities. While typically the calculation of an anisotropic Fermi surface realted physical property requires the consideration several thousand points on the surface, say in an impurity or Boltzmann transport problem, the Helmholtz Fermi Surface harmonics (HFSH) technique allows us to accurately treat these problems considering few elements of the HFSH set. Here we introduce the recent developments in this direction, including the symmetry treatment and derived selection rules, and a representative benchmarking list of examples illustrating the potential of this method.