O 17: Mini-Symposium: Frontiers of electronic-structure theory: Focus on electron-phonon interactions I

Time: Monday 13:30–15:30 Location: R3

Invited Talk O 17.1 Mon 13:30 R3

Predominance of non-adiabatic effects in zero-point renormalization of electronic energies — •Xavier Gonze[1,2], Anna Miglio[1], Véronique Brousseau-Couture[3], Gabriel Antonius[4,5], Yang-Hao Chan[4], Steven Louie[4], Bogdan Guster[1], Matteo Giantomassi[1], and Michel Côté[3] — [1]UCLouvain, Belgium — [2]Skoltech, Moscow, Russia — [3]U. de Montréal, Canada — [4]U. California at Berkeley, USA and NBNL, Berkeley, USA — [5]U. Québec à Trois-Rivières, Canada

Electronic and optical properties of materials are affected by atomic motion through electron-phonon interaction: not only band gaps change with temperature, but even at zero K, zero-point motion causes band-gap renormalization. We present a large-scale first-principles evaluation of the zero-point renormalization beyond the adiabatic approximation [1]. For materials with light elements, the band gap renormalization is often larger than 0.3 eV, and up to 0.7 eV. This effect cannot be ignored if accurate band gaps are sought. For infrared-active materials, global agreement with available experimental data is obtained only when non-adiabatic effects are taken into account. They even dominate zero-point renormalization for many materials, as shown by a generalized Fröhlich model that includes multiple phonon branches, anisotropic and degenerate electronic extrema, whose range of validity is established by comparison with first-principles results. We also investigate effective mass changes in such generalized Fröhlich model. [1] A. Miglio et al. npj Computational Materials, 6, 167 (2020).

Invited Talk O 17.2 Mon 14:00 R3

Huge quantum effects on the 250 K superconducting lanthanum hydride — •Ion Errea — University of the Basque Country, San Sebastian, Spain

The discovery of superconductivity at 200 K in the hydrogen sulfide system at large pressures was a clear demonstration that hydrogen-rich materials can be high-temperature superconductors. The recent synthesis of LaH10 with a superconducting critical temperature (Tc) of 250 K place these materials at the verge of reaching the long-dreamed room-temperature superconductivity. Here we show that quantum atomic fluctuations stabilize in the superconducting pressure range a high-symmetry Fm-3m crystal structure consistent with experiments, which has a colossal electron-phonon coupling of 3.5. Even if ab initio classical calculations predict this structure to distort below 230 GPa yielding a complex energy landscape, the inclusion of quantum effects evidences the Fm-3m as the true ground state. The agreement between the calculated and experimental Tc values further supports this phase as responsible for the 250 K superconductivity. The relevance of quantum fluctuations questions many of the crystal structure predictions made for hydrides within a classical approach that at the moment guide the experimental quest for room-temperature superconductivity. Furthermore, quantum effects are revealed to be crucial to stabilize solids with extraordinary electron-phonon coupling, which may otherwise be destabilized by the large electron-phonon interaction, reducing the pressures needed for their synthesis.

Invited Talk O 17.3 Mon 14:30 R3

Out-of-equilibrium lattice dynamics in two-dimensional materials — •Fabio Caruso — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel

The coupling between electronic and vibrational degrees of freedom influences profoundly the ultrafast dynamics of electrons [1] and phonons [2]. We conducted first-principles calculations of the coupled electron-phonon dynamics to investigate the characteristic fingerprints of crystal-lattice vibrations in systems driven out of equilibrium by the interaction with ultra-short light pulses. The relaxation of photo-excited carriers via phonon emission exhibits a striking selectivity in momentum space, and it underpins the emergence of a non-thermal vibrational state of the lattice. These vibrational excited states are characterized by a highly anisotropic population of different phonons and persist for up to 10 ps, until thermal equilibrium is re-established by phonon-phonon scattering. For the prototypical layered semiconductors black phosphorus and MoS2, these findings are corroborated by femto-second electron diffuse scattering (FEDS) experiments [3]. The control of non-thermal vibrational states may provide unexplored opportunities to selectively enhance the phonon population and, thereby, transiently tailor electron-phonon interactions over picosecond time scales.

[1] Caruso, Novko, Draxl, Phys. Rev. B 101, 035128 (2020). [2] Novko, Caruso, Draxl, Cappelluti, Phys. Rev. Lett. 124, 077001 (2020). [3] Seiler, Zahn, Zacharias, Hildebrandt, Vasileiadis, Windsor, Qi, Carbogno, Draxl, Caruso, Ernstorfer, arXiv:2006.12873 (2020).

Invited Talk O 17.4 Mon 15:00 R3

Ultrafast optical control of complex oxide functional properties: New insights from theory and first-principles calculations — •Nicole Benedek — Cornell University, Ithaca, NY USA

Recent experiments have demonstrated the potential for ultrafast changes in the functional properties of materials upon selective optical excitation of particular phonon modes. The chemical diversity of complex oxides, and their strong lattice-properties coupling, have made them ideal test systems for new experimental approaches that exploit anharmonic phonon couplings to induce and modify magnetism, superconductivity and ferroelectricity with light. In this talk, I will describe our recent theoretical efforts exploring ultrafast optical control of the functional properties of perovskite oxides. First, I will describe the theoretical framework that we have developed, and the role of electronic structure calculations in that framework. I will then focus on an example of our framework in action: dynamical stabilization of a non-equilibrium magnetic phase in $GdTiO_3$. Finally, I will consider how to identify materials that may exhibit a large dynamical response and present our results of a systematic exploration of intrinsic materials factors that may contribute to the nonlinear phononics response in $LaAlO_3$. Our work highlights the importance of understanding the contributions of small structural distortions to the optical response in perovskites (in contrast with large-amplitude distortions, such as octahedral rotations), and illustrates how anharmonic mode coupling strengths may not be the most important factor in which materials exhibit large or unusual responses, as has generally been assumed.