O 96: Poster Session VII: Poster to Mini-Symposium: Frontiers of electronic-structure theory IV

Time: Thursday 10:30–12:30 Location: P

O 96.1 Thu 10:30 P

Electronic structure of β-SiAlON: effect of Al/O doping and of finite temperature — •Saleem Ayaz Khan[1], Ondrej Sipr[2], Jiri Vackar[2], Robin Niklaus[3], Peter J Schmidt[4], Wolfgang Schnick[3], and Jan Minar[1] — [1]University of West Bohemia, Czech Republic — [2]Institute of Physics of the Czech Academy of Sciences — [3]LMU Munich, Germany — [4]Lumileds Development Center, Aachen, Germany

Electronic structure of a series of ordered and disordered β-$Si_{6-z}Al_zO_zN_{8-z}$ systems is investigated by means of ab initio calculations, using the FLAPW method as implemented in the wien2k code and Green function KKR method as implemented in the spr-kkr code. Finite temperature effects are included within the alloy analogy model. We found that the trends with the Al/O doping are similar for ordered and disordered structures. The electronic band gap decreases with increasing z by about 1 eV when going from z=0 to z=2. The optical gap decreases analogously as the electronic band gap. The changes in the density of states (DOS) at Si and N atoms introduced by doping β-Si_3N_4 with Al and O are comparable to the DOS at Al and O atoms themselves. The bottom of the conduction band in β-$Si_{6-z}Al_zO_zN_{8-z}$ is formed by extended states residing on all atomic types. Increasing the temperature leads to a shift of the bottom of the conduction band to lower energies. The amount of this shift increases with increasing doping z.

O 96.2 Thu 10:30 P

A Bethe-Salpeter equation and a GW approach with electron-phonon coupling: from exciton binding energies to charge mobilities. — •Paolo Umari — University of Padova, Padova, Italy

e have introduced a simple scheme in order to account for the coupling with longitudinal phonons within the first-principles Bethe-Salpeter approach based on many-body perturbation theory. This allows to evaluate the reduction of exciton binding energies observed in polar semiconductors. The electron-phonon coupling is modelled from the macroscopic dielectric response in the infrared which, in turn, is calculated through density functional perturbation theory. In this way, the additional computational cost determined by our method is negligible. I will first illustrate our approach in the case of bulk ZnS and show how the excitonic series of bulk Cu2O is well reproduced[1]. The method could clarify the role of dielectric screening in hybrid perovskites yielding exciton binding energies in agreement with experiment[2]. Finally, I will discuss the extension of our method to GW calculations and I will show how the renormalisation of band-gaps and effective masses, and electron and hole mobilities can be easily calculated. Results for the hybrid perovskite MAPbI3 are in agreement with the most accurate calculations which include explicitly the coupling with phonons.

[1]L. Adamska and P. Umari, Phys. Rev B accepted (2021) [2]P. Umari, E. Mosconi, F. De Angelis, J. Phys. Chem. Lett. 9, 620 (2018).

O 96.3 Thu 10:30 P

Sticking coefficient for atoms scattering off metallic surfaces — •Celso Ricardo Caldeira Rego — Institute of Nanotechnology KIT

Achieving a complete understanding of the quantum dynamical processes arising when an atom approaches a metallic surface remains a challenge in surface physics. Conventional approaches based on the Born-Oppenheimer approximation become inapplicable when some charge is transferred between the surface and the adatom, and the resulting image-charge potential accelerates the particle towards the surface. Here, we solve the time-dependent Schrödinger equation to compute the electronic contribution to the sticking coefficient for a generalized version of the Anderson-Newns Hamiltonian and obtain adsorption probabilities as large as 15%. Numerical simulations demonstrate that the creation of low-energy electron-hole pairs is an efficient dissipation mechanism that may absorb kinetic energy from the incident particle to cause adsorption. The recently proposed exact-factorization formalism affords a physical interpretation of the results.

O 96.4 Thu 10:30 P

The electron-phonon scenario of superconductivity of LiBi — •Sylwia Gutowska[1], Bartłomiej Wiendlocha[1], Karolina Górnicka[2], Michał Winiarski[2], Weiwei Xie[3], Robert J. Cava[4], and Tomasz Klimczuk[2] — [1]AGH University of Science and Technology in Krakow, Poland — [2]Faculty of Applied Physics and Mathematics, Gdansk University of Technology, ul. Narutowicza 11/12, 80-233 Gdańsk, Poland — [3]Department of Chemistry, Louisiana State University, Baton Rouge Louisiana 70803, United States — [4]Department of Chemistry, Princeton University, Princeton, New Jersey 08544, United States

The electron-phonon interaction scenario of superconductivity is investigated in case of LiBi, which is a compound made of the lightest and the heaviest elemental metal and which hosts the tetragonal structure with squared sublattices of Bi, unusual for Bi-based compounds, that prefer the hexagonal type of sublattices due to the 3 valence electrons of 6p nature of bismuth. Such a simple structure is a perfect candidate for an investigation in details of the influence of the electronic as well as the phonon structure on the electron-phonon interaction and the superconductivity. After that, we compare the results in terms of electron-phonon coefficient and critical temperature to the experimental values. We also study the isotope effect and the influence of external pressure on the structure and superconductivity of this compound.

O 96.5 Thu 10:30 P

Energy gap closure of crystalline molecular hydrogen with pressure — •Vitaly Gorelov[1], Markus Holzmann[2,3], David M. Ceperley[4], and Carlo Pierleoni[1,5] — [1]Université Paris-Saclay, UVSQ, CNRS, CEA, Maison de la Simulation, Gif-sur-Yvette, France — [2]Univ. Grenoble Alpes, CNRS, LPMMC, Grenoble, France — [3]Institut Laue-Langevin, Grenoble, France — [4]Department of Physics, University of Illinois Urbana-Champaign, USA — [5]Department of Physical and Chemical Sciences, University of L*Aquila, L*Aquila, Italy

We study the gap closure with pressure in Phases III and IV of molecular crystalline hydrogen. Nuclear quantum and thermal effects are considered from first principles with Coupled Electron Ion Monte Carlo. The fundamental electronic gaps are obtained from grand-canonical Quantum Monte Carlo methods properly extended to quantum crystals. Nuclear zero point effects cause a large reduction in the gap ($\sim$2eV). As a consequence the fundamental gap closes at 530GPa for ideal crystals while at 360GPa for quantum crystals. Since the direct gap remains open until * 450GPa, the emerging scenario is that upon increasing pressure in phase III (C2/c-24 crystal symmetry) the fundamental (indirect) gap closes and the system enters into a bad metal phase where the density of states at the Fermi level increases with pressure up to $\sim$450GPa when the direct gap closes. Our work partially supports the interpretation of recent experiments in high pressure hydrogen.

O 96.6 Thu 10:30 P

gauge-covariant derivatives of the Berry curvature and orbital moment by Wannier interpolation — •Xiaoxiong Liu[1], Miguel Ángel Herrera[2], Stepan Tsirkin[1], and Ivo Souza[2] — [1]Department of Physics, University of Zurich — [2]Centro de Física de Materiales, Universidad del País Vasco

The momentum-space derivatives of the Berry curvature Ω and intrinsic orbital magnetic moment m of the Bloch states arise in multiple problems, such as the nonlinear anomalous Hall effect [1] and magneto-transport within the Boltzmann-equation formalism [2]. To study them from first principles, we developed a Wannier interpolation scheme for evaluating "generalized derivatives" of the non-Abelian Ω and m matrices for a group of bands of interest.

The generalized derivative does not involve couplings within the group, and preserves the gauge covariance of the Ω and m matrices. This formulation leads to robust *Fermi-sea* formulas for the Berry curvature dipole [1] and kinetic magnetoelectric effect tensor [2], which converge much faster with the density of the integration k-grid than the *Fermi-surface* formulas implemented earlier [3] in the Wannier90 code. The implementation is done in our newly-developed code WannierBerri [4]. We demonstrate the method with ab initio calculations on real materials, as well as tight-binding toy models.

[1] Sodemann et al, PRL 115 (2015): 216806.
[2] Zhong et al, PRL 116 (2016): 077201.
[3] Tsirkin et al, PRB 97 (2018): 035158.
[4] wannier-berri.org

O 96.7 Thu 10:30 P

Soft-mode enhanced type-I superconductivity in $LiPd_2Ge$

— •Gabriel Kuderowicz[1], Karolina Górnicka[2], Elizabeth M. Carnicom[3], Kamil Kutorasiński[1], Tomasz Klimczuk[2], Robert J. Cava[3], and Bartłomiej Wiendlocha[1] — [1]Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Aleja Mickiewicza 30, 30-059 Kraków, Poland — [2]Faculty of Applied Physics and Mathematics and Advanced Materials Centre, Gdansk University of Technology, Narutowicza 11/12, 80-233 Gdańsk, Poland — [3]Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA

Recently synthesized intermetallic compound $LiPd_2Ge$ exhibits superconductivity below T_c=1.96 K. It belongs to the Heusler family which consist of more than 1000 compounds with various kinds of physical properties. Following the discovery of $LiPd_2Ge$ we synthesized isostructural and isoelectronic $LiPd_2Si$ and $LiPd_2Sn$. In this work we present DFT calculations of electronic structure, phonons and electron-phonon coupling. All three compounds have strong softening of the first acoustic mode. $LiPd_2Ge$ has mostly pronounced softening and the highest value of the electron-phonon coupling constant $\lambda = (0.53 - 0.56)$ and highest T_c. Therefore, we suggest the correlation between superconductivity and the soft mode. We were looking for sources of phonon instabilities and observed deviations from harmonic potential.