DY 50 Lattice Dynamics and Non-Linear Excitations

Time: Friday 10:15–11:30 Room: HÜL 186

DY 50.1 Fri 10:15 HÜL 186

Continuous time quantum Monte-Carlo simulations of polarons and bipolarons — •J.P. Hague[1], P.E. Kornilovitch[2], A.S. Alexandrov[1], and J.H. Samson[1] — [1]Dept. of Physics, Loughborough University, LE11 3TU, UK — [2]Hewlett-Packard Company, 1000 NE Circle Blvd, Corvallis, Oregon 97330, USA

We present the results of a continuous-time quantum Monte-Carlo algorithm for simulating polarons and bipolarons. An exact integration over phonon degrees of freedom leads to an efficient algorithm, which may be used for arbitrary interaction range. We consider the effects of lattice geometry and dimensionality on polaron properties including the effective mass, energy, number of phonons involved in the polaron, mass isotope coefficient, polaron spectrum and polaron density of states. In particular, we find that the coordination number has a greater effect on the polaron dynamics than the dimensionality, and that long-range Fröhlich interactions wash-out the effects of the lattice geometry (cond-mat/0509590). Finally, we discuss extensions of the algorithm to simulate bipolarons on various lattice configurations (e.g. the staggered ladder).

DY 50.2 Fri 10:30 HÜL 186

Phonons at the β-tin→*Imma*→sh phase transitions in Si: An *ab-initio* study — •Katalin Gaal-Nagy — Dipartimento di Fisica, Universita degli Studi di Milano, Via Celoria 16, 20133 Milano (Italy)

We present an ab-initio study of the lattice statics and dynamics of Si near the β-tin→*Imma*→ sh phase transitions. Our results allow a new interpretation of measured Raman phonon frequencies of what was thought to be the β-tin phase. A comparison of our data with the experimental ones shows that the phase transitions β-tin→*Imma*→sh have been already indicated in the Raman spectra even though not realized because of marginal changes. Furthermore, we find a soft-mode behavior for the phase transition sh→*Imma*. The transition pressure for the β-tin→*Imma* phase transition can be determined precisely from the phonon frequencies rather than from the lattice parameters. This work has been performed using the plane-wave pseudopotential approach to the density-functional theory and the density-functional perturbation theory within the local density approximation.

DY 50.3 Fri 10:45 HÜL 186

Soft local phonon modes in thermoelectric materials — •Werner Schweika[1] and Raphael Hermann[2] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, 52425 Jülich — [2]Department of Physics, B5, University of Liege, Belgium

We have studied powders of three different thermoelectric materials, Tl-filled skutterudites[1], Ba- and Sr-filled germanium clathrates[2], and Zn4 Sb3 alloys, by inelastic neutron scattering. For all materials, a common feature of a prominent soft local phonon mode with an energy of about 5 meV has been observed consistently with Einstein modes of rattling atoms in these relatively open cage-like structures. While approaches to thermoelectric properties often focus on the electronic structure our results indicate that local phonon modes play a key role in providing an effective scattering mechanism for the heat transporting acoustic phonons.

[1] Phys. Rev. Lett. 90, 135505-1 (2003).
[2] Phys. Rev. B 72, 174301 (2005).

DY 50.4 Fri 11:00 HÜL 186

Raman spectroscopy studies on THF clathrate hydrates — •Beata Walasek, Sascha Eschborn, and Rudolf Feile — Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstr. 8, 64289 Darmstadt

Clathrate hydrates consist of an ice-like tetrahedral network of hydrogen bonded water molecules, forming polyhedral cages in which various guest molecules can be enclosed. The host lattice is stabilised by van der Waals interaction between guest and water molecules.

We investigate the interaction of tetrahydrofurane (THF) molecules with the host water cage comparing THF molecular vibrations in pure THF with those of THF molecules in the neighbourhood of either water molecules in liquid water or water molecules forming the clathrate cages. Raman spectra of aqueous and deuterated water solutions of THF were recorded from 500 cmˆ-1 to 3500 cmˆ-1 The strongest influence of the THF-water interaction is observed for the ring breathing mode (C-C-C-C stretches) and C-O-C stretch mode around 920 cm-1. In pure THF both vibrational modes have almost the same frequency. The interaction (hydrogen bonding) with H_2O/D_2O shifts the C-O-C mode in liquid water. On formation of the clathrate both vibrations have almost the same frequency again, showing that the hydrogen bonds of the THF molecule to neighboring H_2O/D_2O molecules are strongly weakened in the clathrate.

Below 120 K a splitting of the two modes set in. This may reflect either structural changes in the host lattice or the freezing of the THF molecule into inequivalent orientations within the cage.

DY 50.5 Fri 11:15 HÜL 186

Stability limits for CuAu phase of $CuInS_2$ — •Jan Łaźewski and Krzysztof Parlinski — Institute of Nuclear Physics Polish Academy of Sciences, Radzikowskiego 152, 32-342 Kraków, Poland

The ternary chalcopyrite compounds $CuInX_2$ (X=S,Se) and its alloys are promising semiconductor materials with practical application as stable and radiation resistant polycrystalline thin film photovoltaic solar cells with power conversion efficiencies increasing steadily over the years. One of the interesting features of these materials is high contamination of chalcopyrite structure with nearly isenthalpic CuAu-structure.

We present the results of a comparative first-principles calculation of the structure parameters and the lattice dynamical properties for the CuAu-ordered and chalcopyrite phases of $CuInS_2$. The frequencies and symmetries of five optical phonon modes are determined for $CuInS_2$ with CuAu-ordered structure. We have found very small difference between the total energies of both structure types at elevated temperatures according to our calculations. The frequency range covered by the zone-center vibrational modes, the phonon dispersion, and the phonon density of states are very similar for both structure types. Furthermore, the frequencies of the infrared modes of the CuAu-ordered phase deviate only slightly from mode frequencies observed for the chalcopyrite phase. The only exception is the fully symmetric A1 mode having a distinctly higher frequency in CuAu-ordered $CuInS_2$.

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