MM 30: Complex Materials

Time: Wednesday 16:15–17:15 Location: IFW D

MM 30.1 Wed 16:15 IFW D

Numerical solutions of the elastodynamic equations for icosahedral quasicrystals — •Frohmut Rösch and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany

The vibrational properties of most solids can be characterized by the time evolution of the phononic displacements $\mathbf{u}(\mathbf{x},t)$. In quasicrystals, however, additional degrees of freedom must be taken into account, which are described by the so-called phasonic displacements $\mathbf{w}(\mathbf{x},t)$. The latter are related to flips of atoms in the atomic picture.

The governing equations, which describe the dynamic behavior of both $\mathbf{u}$ and $\mathbf{w}$, are extensions of the elastodynamic equations for crystals generalized by the phasonic degrees of freedom. These result in propagating (phonon-like) and diffusive (phason-like) elementary modes.

A finite element package has been adjusted to solve the elastodynamic equations for a three-dimensional icosahedral quasicrystal. Fundamental scenarios, e.g. the time evolution of phason and phonon excitations in a finite sample, are investigated and compared to analytic solutions.

MM 30.2 Wed 16:30 IFW D

Effective potentials for phonon dynamics in clathrates — •Daniel Schopf and Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany

Intermetallic clathrates are currently actively investigated due to their special thermoelectric properties. They are composed of periodically arranged cages, formed by host atoms, which enclose single guest atoms. The low thermal conductivity of these structures has been attributed to the interaction of the phonons with local vibration modes ("rattling") of these guest atoms inside the host framework.

For computational studies of dynamic properties long simulation times and large samples are required. This makes first principle calculations of these structures, even with very fast computers, very unfeasible. Classical molecular dynamics, however, can easily handle large systems and long simulation times. The potentials needed for these MD simulations can be obtained from ab-initio calculations with the force-matching method. It uses large numbers of reference data to fit an effective potential that can reproduce the forces, energies and stresses of the ab-initio calculation.

To model the strongly directional atomic interactions in clathrates, angular dependent potentials are required. An analytic potential will be presented to model these systems. The phonon dynamics of clathrates was studied with these potentials and will be compared with ab initio results.

MM 30.3 Wed 16:45 IFW D

Eigenstates and electronic transport in the generalized Labyrinth tiling — •Stefanie Thiem and Michael Schreiber — Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

Understanding the physical properties of quasicrystals requires a deeper insight into the nature of the eigenstates of these systems and their relation to the transport properties. We present results for d-dimensional quasiperiodic models based on the metallic mean sequences constructed by the inflation rule $\mathcal{P}_a = \{x \to y, y \to yxy^{a-1}\}$, where x and y denote the strengths of the two bond types. The eigenstates of the quasiperiodic chain are obtained by numerical diagonalization of the tight-binding Hamiltonian. Higher dimensional solutions of the associated generalized labyrinth tiling are constructed then by a product approach from the one-dimensional eigenstates, allowing the numerical consideration of large systems up to 10^{11} sites. Thereby, we obtain information about the localization of the wave functions by investigating the scaling behavior of the participation ratio and about the electronic properties by studying the scaling behavior of the wave packet spreading with time. We present results for different scaling exponents and investigate their relations in order to obtain a better understanding of the characteristics of quasicrystals.

MM 30.4 Wed 17:00 IFW D

Order Parameter Dynamics in the quasi two-dimensional Charge Density Wave System $2H-TaSe_2$ — •Tim Huber[1], Hanjo Schäfer[1], Helmuth Berger[2], and Jure Demsar[1] — [1]Physics Department, Universität Konstanz,78457, Germany — [2]Institut de Physique de la Matiere Complexe, EPFL, 1015 Lausanne, Switzerland

Recent results of time-resolved spectroscopy on the quasi one-dimensional charge density wave (CDW) system $K_{0.3}MoO_3$ have shown that on a short timescale, the electronic and lattice parts of the CDW order parameter are disentangled (Schäfer et al., PRL 105, 066402 (2010)). Here we present the data on the quasi two-dimensional CDW system $2H-TaSe_2$ and show - utilizing a time-dependent Ginzburg-Landau model - that they can be interpreted within the same theoretical framework. We demonstrate that also in the quasi two-dimensional case, the appearance of low frequency Raman active modes and their T-dependence can be naturally explained by linear coupling of the electronic part of the order parameter to the $2k_f$ phonons. Compared to $K_{0.3}MoO_3$, however, in $2H-TaSe_2$ the electronic part of the order parameter faster follows the lattice, demonstrated by stronger mode softening as T_c is approached. In addition, we present the first study on Cu-intercalated $2H-TaSe_2$ which shows a dramatic increase in the CDW transition temperature compared to its parent compound.