TT 27 Solids at Low Temperature - New Materials

Zeit: Dienstag 12:00–12:30 Raum: TU H3027

TT 27.1 Di 12:00 TU H3027

Wigner crystallization in $Na_3Cu_2O_4$ and $Na_8Cu_5O_{10}$ chain compounds — •P. Horsch, M. Sofin, M. Mayr, and M. Jansen — Max-Planck-Institut fuer Festkoerperforschung, D-70569 Stuttgart, Germany

We report the synthesis of novel edge-sharing chain systems $Na_3Cu_2O_4$ and $Na_8Cu_5O_{10}$, which form insulating states with commensurate charge order. We identify these systems as one-dimensional Wigner lattices, where the charge order is determined by long-range Coulomb interaction and the number of holes in the d-shell of Cu. Our interpretation is supported by X-ray structure data as well as by an analysis of magnetic susceptibility and specific heat data. Remarkably, due to large second neighbor Cu-Cu hopping, these systems allow for a distinction between the (classical) Wigner lattice and the $4k_F$ charge-density wave of quantum mechanical origin.

TT 27.2 Di 12:15 TU H3027

Influence of structural distortions on electronic properties of Ba_6Ge_{25} clathrate — •Ivica Zerec[1], Wilder Carrillo-Cabrera[1], Vladimir Voevodin[1], Jörg Sichelschmidt[1], Alexander Yaresko[2], Peter Thalmeier[1], and Yuri Grin[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden — [2]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden

Clathrates are cage compounds, recently investigated as interesting candidates for thermoelectric applications. The complex structure poses a major challenge in understanding the variety of their interesting physical properties. We present the electronic band structure calculations for Ba_6Ge_{25} clathrate. It undergoes an involved structural phase transition, accompanied with stepwise changes of many physical quantities. We construct the ordered structural models for different temperatures, in accordance with the experimental data and calculate the corresponding electronic band structures. We show how the changes of electronic properties across the phase transition may be understood from the modifications of the band structure induced by the structural distortions. In particular we show how the shift of the optical spectral weights towards higher frequencies, observed in the optical conductivity below the phase transition, is well reproduced by the theoretical calculations based on the electronic band structure.