Stuttgarter Physikalisches Kolloquium

Max-Planck-Institut für Festkörperforschung
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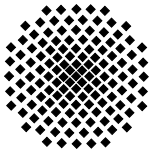

Dienstag, 15. Januar 2019 | **16.15 Uhr** | **Hörsaal 2D5**

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An effective molecular orbital approach to electron phonon and pairing interactions in skipped valence and (negative) charge transfer gap Oxides

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Abstract

In high oxidation state oxides like the trivalent Nickel oxides, tetravalent Co and Fe oxides as well as the parent superconductors BaBiO3 and SrBiO3 and High Tc hole doped cuprates, the cation electron affinity in the formal valence could end up larger than the O 2- ionization potential leading to a so called negative charge transfer gap. If the charge transfer energy is strongly negative, then we should really adopt starting electronic configurations such as Ni2+ rather than 3 + or Bi 3+ rather than 4+ with compensation holes in the O 2p valence band for charge neutrality. If in addition the lowest energy cation ionization states are strongly hybridized with the valence O 2p states the low energy scale electronic structure and be well described by a molecular orbital type of approach.

This is a new approach to the Wannier function description but with explicit inclusion of the O states which provides a natural path to inclusion of the electron phonon coupling, charge density wave formation, potential bipolaron formation and paring interactions in superconductors. We discuss recent developments in this approach and show that the effective electron phonon coupling involving these molecular like orbitals is much stronger than that estimated from density function approaches. We also show that this leads to Peierls like charge density wave like ground states and we describe how the electron phonon coupling involving the hopping integrals rather than the on-site energies evolves into a large effective attractive interaction between low energy scale electrons. I will also briefly describe how these effects lead to our coelution that the ion battery material LiNiO2 should be viewed as an “entropy-stabilized charge- and bond-disproportionated glass”.