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Friedrich Roth

Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden

Electronic structure of selected aromatic hydrocarbon systems investigated with electron energy-loss spectroscopy

Organic materials with fascinating/intriguing electronic properties have been the driving force for many research activities in the past, and in particular for important progress in materials science covering both new functional materials as well as theoretical developments. In addition, charge transfer, i. e., the addition or removal of charges to or from molecules in organic solids is one route to modify and control their electronic properties. Recently, the discovery of superconductivity in several alkali metal intercalated hydrocarbon systems (picene, phenanthrene, coronene and 1,2;8,9-dibenzopentacene) with rather high transition temperatures has opened a new chapter in organic material science as well as solid-state physics.

The search for a microscopic understanding of the mechanism that drives materials superconducting always has initiated a large number of scientific activities, and there are numerous examples where these activities have provided major advancement. A basic foundation of this understanding is the knowledge of the electronic properties of the material under investigation. In this context, the talk presents first, very detailed insights into the electronic structure of both undoped as well as potassium doped picene and 1,2;8,9-dibenzopentacene using electron energy-loss spectroscopy (EELS) as main experimental method. In order to learn more about the electronic structure we have compared the results we obtained from EELS with theoretical calculations based on Density functional theory (DFT) using the local-density approximation (LDA). Finally, investigations of the electronic properties of undoped and potassium doped chrysene, a close relative of picene, show that the doping introduced changes are in a similar range such as observed in case of picene. Interestingly, due to the analogy between the observed changes in the electronic structure upon potassium doping between chrysene and picene and further similarity in the crystal structure we speculate that chrysene is a promising candidate for another aromatic hydrocarbon superconductor.

Host: Wolfgang Eberhardt, CFEL UNI-ASG Seminar