Transport and charge transfer in metal phthalocyanine hetero structures: theoretical aspects and applications

T. Hahn[a], J. Kortus[a], F. Rückerl[b] , P. Siles[c] and M. Knupfer[b]

[a]TU Bergakademie Freiberg, Leipziger Str. 23, D-09596 Freiberg, Germany
[b]Institute for Solid State Research, IFW Dresden, D-01171 Dresden, Germany
[c]Institute for Integrative Nanosciences, IFW Dresden, D-01171 Dresden, Germany

Novel charge-transfer compounds formed by combining Metal-Phthalocyanines with different acceptor molecules offer a large variety of physical phenomena and potential applications. Due to the importance of phthalocyanine compounds for fundamental research as well as for future applications it is essential to understand how to modify their electronic properties.

We will present the results of our theoretical first-principle investigations on selected organic charge transfer materials. In particular, we will discuss methodic details about the calculation of charge transfer on pure organic interfaces as well as on organic / metal hetero structures. Further we discuss the implications of charge and spin state changes for typical transport experiments. Such well-controlled tuning of the electrical properties of phthalocyanine junctions stands as key step for future phthalocyanine-based electronic devices. Finally, we will briefly introduce a methodical enhancement to the Density Functional Theory framework that possibly enables the further quantitative description of charge transfer.

This work has been supported by the Deutsche Forschungsgemeinschaft within the Research Unit FOR 1154.

Keywords: Density Functional Theory, Charge transfer, Electronic Structure, Quantum Transport