Institut für Physik
Montanuniversität Leoben
A-8700 LEOBEN, Franz Josef Straße 18, Austria
Tel: +43 3842 402-4601, Fax:+43 3842 402-4602
e-mail: physics@unileoben.ac.at

SEMINAR
aus
Halbleiterphysik und Nanotechnologie

Di, 16.5.2017, 11:00 Uhr, Hörsaal für Physik

"Electrostatic Design of Low-Dimensional Organic Materials"

Ao.Univ.-Prof. Dipl.-Ing. Dr.techn. Egbert Zojer
Institute of Solid State Physics, Graz University of Technology, NAWI Graz, Graz, Austria

For realizing the promises of organic nano-electronics it is crucial to control the nature of the electronic states within the materials as well as at interfaces. This is commonly achieved through functional chemical substitutions that tune the properties of individual molecules. Deviating from that approach, we here portray a largely unexplored strategy that exploits collective electrostatic effects1 arising from the superposition of the electrical fields of assembled polar groups. Such effects typically determine the electronic and transport properties of organic monolayers2 and their consequences are not always advantageous. When employing them in a well-defined manner, they can, however, be used for realizing materials with novel properties, as discussed here on the basis of DFT-type quantum-mechanical simulations.

For example, we use them to develop a modular toolbox for relatively complex organic quantum-systems at interfaces including monolayer-based quantum-cascades, quantum-wells, and locally spin-sensitive molecular films.3 First steps towards an experimental realization of such systems are also discussed.4 Additionally, we address how collective electrostatic effects can be used for tuning the electronic properties of 2D-like electron systems such as graphene, monolayers of hexagonal boron-nitride and layered semiconductors.5 Extending the concepts to bulk materials we, furthermore, propose design strategies for realizing complex organic frameworks, whose properties are determined by a deliberate alignment of polar building blocks. Common to all those cases is a pronounced localization of the frontier electronic states in different spatial regions of the materials and a shift of their energies, both of which can be controlled by the distribution and value of the used local dipoles.

References

[1] G. Heimel et al. Acc. Chem. Res. 2008, 41: 721; G. Heimel et al. Adv. Mater., 2010, 22: 2494; [2] G. Heimel et al., Phys. Rev. Lett., 2006: 193310; G. Heimel et al., Adv. Mater. 2012, 24: 4403, V. Obersteiner et al., J. Phys. Chem. C 2014, 118: 22395; V. Obersteiner et al., J. Phys. Chem. C, 2015, 119: 21198; T. Taucher et al., J. Phys. Chem. C., 2016: 1328; I. Hehn et al. J. Phys. Chem. Lett., 2016, 7: 2994; [3] B. Kretz et al., Advanced Science, 2015, 1400016; [4] T. Abu-Husein et al., Adv. Funct. Mater., 2015, 25: 3943; A. Kovalchuk et al., Chemical Science, 2016, 7: 718; A. Kovalchuk et al., RSC Adv., 2016, 6: 69479; [5] G. Kraberger et al., Adv. Mater. Interfaces, 2015, 1500323.