Molecular n-Doping of Carbon Allotropes: The Case of C60 fullerenes

Frank Ortmann
C. Gaul, S. Hutsch, S. Schellhammer
Technische Universität Dresden, Center for Advancing Electronics Dresden, 01062 Dresden, Germany

frank.ortmann@tu-dresden.de

Doping of semiconductors is a key technology for conventional semiconductor electronics and will be important for carbon-based materials such as graphene, carbon nanotubes or fullerenes as well.
The dopant interaction with such materials can be large or weak depending on whether the dopants are incorporated in the sp-2 carbon network, chemisorb or physisorb on top of it. Physisorbed molecules have the advantage of perturbing the electronic properties only very weakly [1] thus keeping disorder at a minimum. In this way detrimental effects of doping on the mobility in form of sp-3 defects [2] can be avoided.
Here we develop a comprehensive doping model and study the doping efficiency of a set of molecular n-type dopants (radical-dimers, organometallics etc.) for the semiconducting C60 fullerene [3]. We relate the doping induced gap states to characteristic doping energies and predict the density of states as well as the pinning/de-pinning behaviour of the Fermi level. We find a very good agreement with experimental photoemission experiments. In addition, we compare our results to transport measurements of doped films, which indicates predictive power of the model for the conductivity.

References

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[3] C. Gaul, S. Hutsch, M. Schwarze, S. Schellhammer, F. Bussolotti, S. Kera, G. Cuniberti, K. Leo, and F. Ortmann, Nat. Mater. (2018); doi: 10.1038/s41563-018-0030-8

Figures

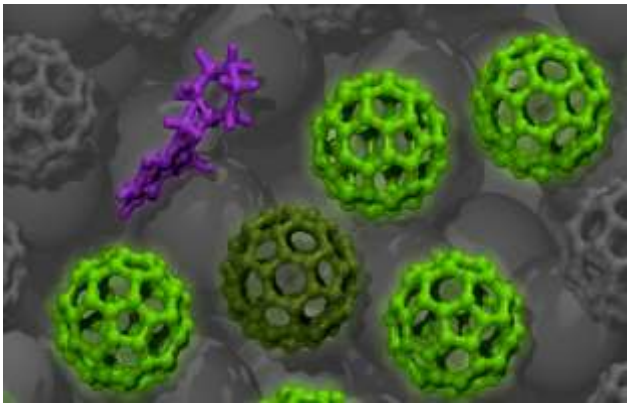

Figure 1: Illustration of a doped organic semiconductor based on fullerene C60 molecules (green). The benzimidazoline dopant (purple) donates an electron to the C60 molecules in its surrounding (dark green). These electrons can then propagate through the semiconductor material (light green).