Tuning the energy levels of organic semiconductors

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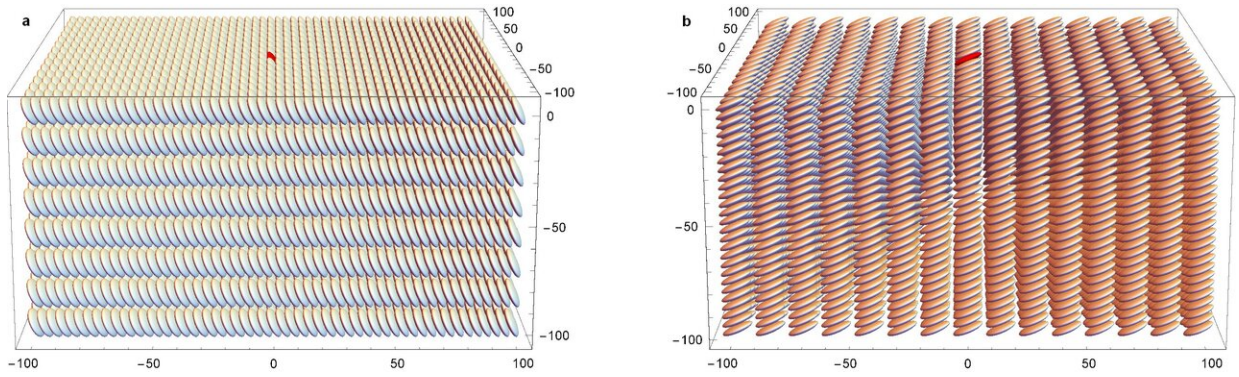

Examples of film structures used for the calculations of the charge - quadrupole interaction energy (EQ) of crystalline films in edge-on (a) and face-on orientation (b). The molecules are represented by discs for illustration purpose. The length scale is given in Å. EQ values are calculated for the red molecules at the film surface. Credit: Frank Ortmann

Physicists from the Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and the Center for Advancing Electronics Dresden (cfaed) at the TU Dresden, together with researchers from Tübingen, Potsdam and Mainz were able to demonstrate how electronic energies in organic semiconductor films can be tuned by electrostatic forces. A diverse set of experiments supported by simulations were able to rationalize the effect of specific electrostatic forces exerted by the molecular building blocks on charge carriers. The study was published

recently in *Nature Communications*.

In electronic devices based on organic semiconductors such as solar cells, light-emitting diodes, photodetectors or transistors, electronic excitations and charge transport levels are important concepts to describe their operation principles and performances. The corresponding energetics, however, are more difficult to access and to tune than in conventional inorganic semiconductors like silicon chips, which stands as a general challenge. This applies both to the measurement and to the controlled influence from outside.

One tuning knob exploits the long-range Coulomb interactions, which is enhanced in organic materials. In the present study, the dependence of the energies of charge transport levels and of excitonic states on blend composition and molecular orientation in the organic material is explored. Excitons are bound pairs of an electron and a hole that are formed in the semiconductor material by light absorption. Scientists refer to blend composition when the components consist of different organic semiconducting materials. The findings demonstrate that the energetics in organic films can be tuned by adjusting a single molecular parameter, namely the molecular quadrupole moment in the pi-stacking direction of the molecules. An electric quadrupole can consist of two positive and two equally strong negative charges which form two oppositely equal dipoles. In the simplest case, the four charges are alternately arranged at the corners of a square.

The authors further link device parameters of organic solar cells such as the photovoltage or the photocurrent to this quadrupole moment. The results help to explain recent breakthroughs of device efficiency in organic solar cells, which are based on a new class of organic materials. As the observed electrostatic effect is a general property of organic materials, including so-called "small molecules" and polymers, it can help to improve the performance of all types of organic devices.

More information: Martin Schwarze et al. Impact of molecular quadrupole moments on the energy levels at organic heterojunctions, *Nature Communications* (2019). DOI: 10.1038/s41467-019-10435-2

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