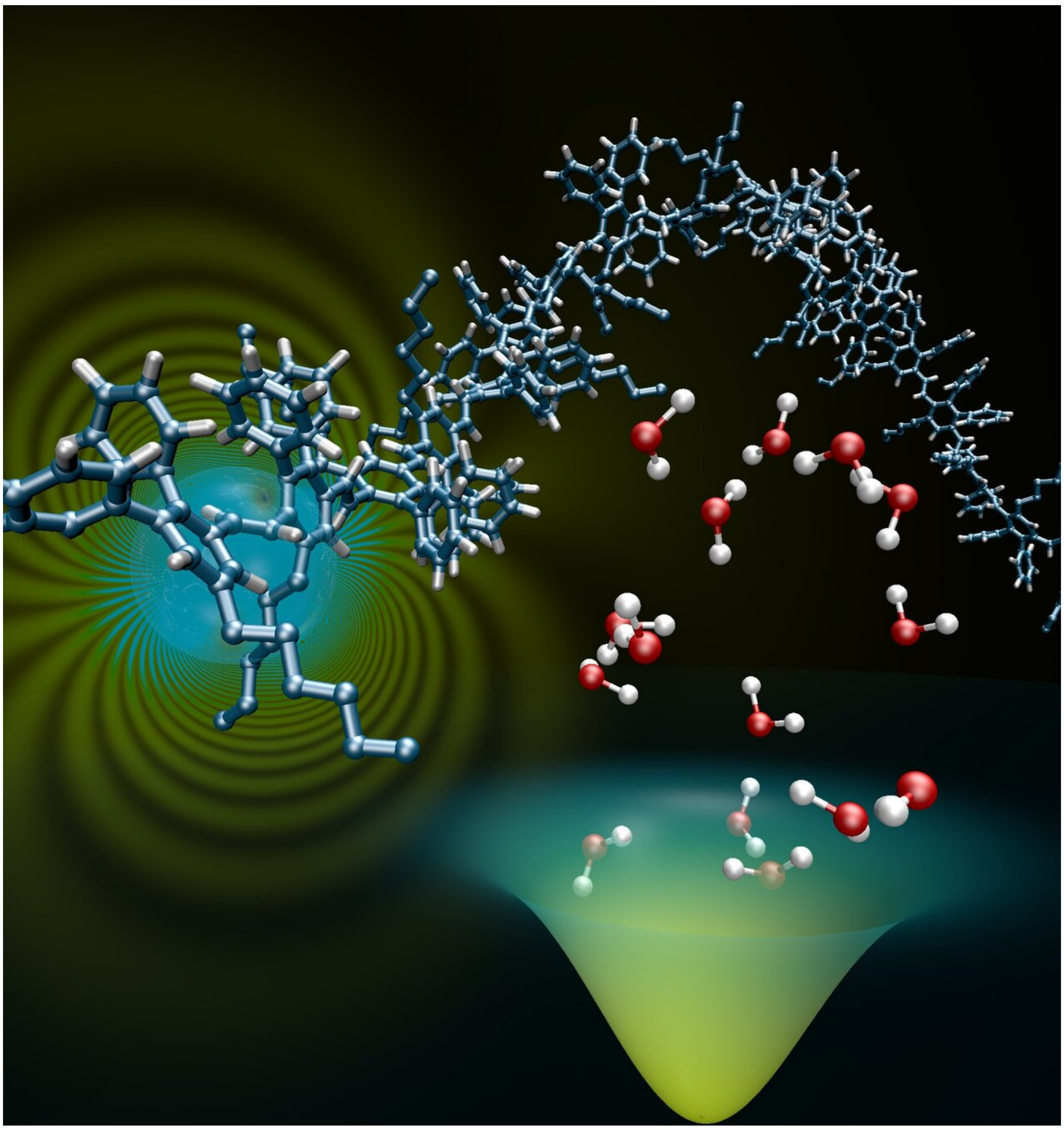
A window for trap-free charge transport in organic semiconductors

October 8 2019, by Ingrid Fadelli



An artist's impression of a cluster of water molecules acting as a hole trap. Credit: D. Andrienko, MPI-P.

Organic semiconductors, a class of carbon-based materials with optical and electronic properties, are now commonly used to fabricate a variety of devices, including solar cells, light-emitting diodes and field-effect transistors. These semiconducting materials can exhibit a characteristic known as highly unipolar charge transport, which essentially means that they predominantly conduct either electrons or holes. This can be somewhat problematic, as it hinders their efficiency and performance.

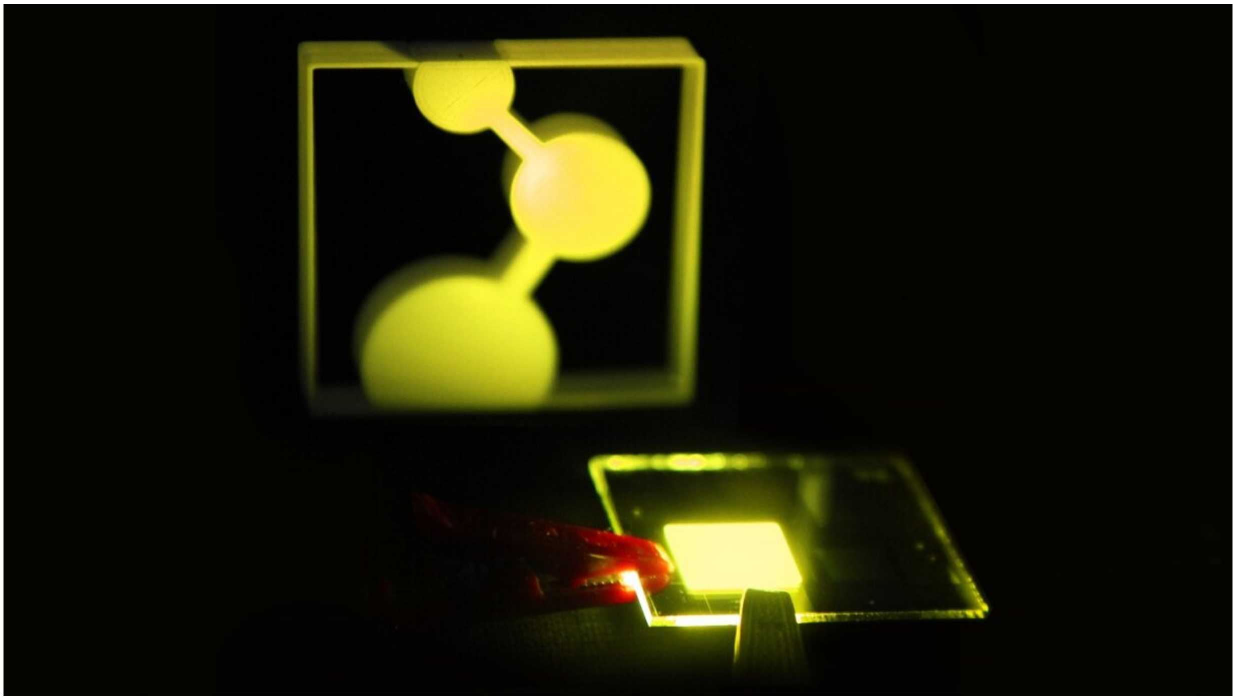
Researchers at the Max Planck Institute for Polymer Research have recently identified an energy window inside which organic semiconductors do not experience charge trapping. As explained in their paper, published in *Nature Materials*, this window enables trap-free charge transport of both carriers.

"In 2012 we investigated the trapping of electrons in conjugated polymers and we found that lowering the energy levels at which electron transport takes place (i.e. LUMO) could reduce the amount of electron trapping," Gert-Jan Wetzelaer, one of the researchers who carried out the study, told TechXplore. "Last year, we developed a strategy to improve the electrodes in organic-semiconductor devices, which allowed us to investigate organic semiconductors with a very large range of energy levels. In our new study, we were interested in how the position of these energy levels would influence the transport of both electrons and holes, even for very deep energy levels, which could previously not be explored."

To investigate how the position of energy levels can influence a semiconductor's ability to transport both electrons and holes, Wetzelaer and his colleagues measured electron and hole currents in a variety of organic semiconductors. In their previous work, they observed that the degree to which this current depends on the voltage applied across a semiconducting film can be used as a measure of the amount of charge trapping.

When the researchers measured the current passing through a large range of organic semiconductors with different energy levels, they found that the energy levels of individual materials influenced whether the current was limited by charge trapping or not. After conducting a series of experiments and gathering numerous observations, they were able to identify a window in which organic semiconductors can achieve trap-free charge transport.

More specifically, they observed that when the ionization energy of a material rises above 6 eV, hole trapping occurs and thus it will no longer be able to efficiently conduct holes. On the other hand, when a material's electron affinity is lower than 3.6 eV, it will not be able to transport electrons efficiently. To effectively conduct both electrons and holes, therefore, a material's ionization and electron affinity energy levels should be within this specific window.



Photograph of the trap-free OLED Credit: MPI-P.

"Our results imply that for optimal performance, the energy levels of the organic semiconductors used in devices, such as OLEDs and organic solar cells, should be ideally situated inside the discovered energy window," Wetzelaer said. "Inside this energy window, the conduction of charge-carriers will be efficient, which is important for converting electricity into light and vice versa."

The study carried out by Wetzelear and his colleagues introduces a general design rule for organic semiconductors that can be used for the fabrication of OLEDs, solar cells and field-effect transistors. This 'general rule' specifies desirable energy levels for achieving higher efficiency and conductivity in devices built using these materials.

"We have recently managed to create a highly efficient OLED based on these design rules, with a much less complex device architecture than normally used," Wetzelaer added.

Wetzelaer and his colleagues carried out a series of simulations and gathered further interesting results, suggesting that water clusters could be the source of hole trapping. This key observation could help to devise strategies to remove charge traps from semiconducting films.

In the future, the energy window identified by this team of researchers could inform the development of more efficient semiconductor-based devices. In addition, their observations raise interesting questions related to the design of blue OLEDs.

"In blue OLEDs, the required energy gap for blue light emission is approximately 3.0 eV, which is larger than the trap-free window," Wetzelaer said. "We are now planning to investigate strategies to remove or disable charge traps in organic semiconductors, to be able to make highly efficient blue OLEDs."

More information: Naresh B. Kotadiya et al. A window to trap-free charge transport in organic semiconducting thin films, *Nature Materials* (2019). DOI: 10.1038/s41563-019-0473-6

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