Physicicists develop new solar cell design for better efficiency

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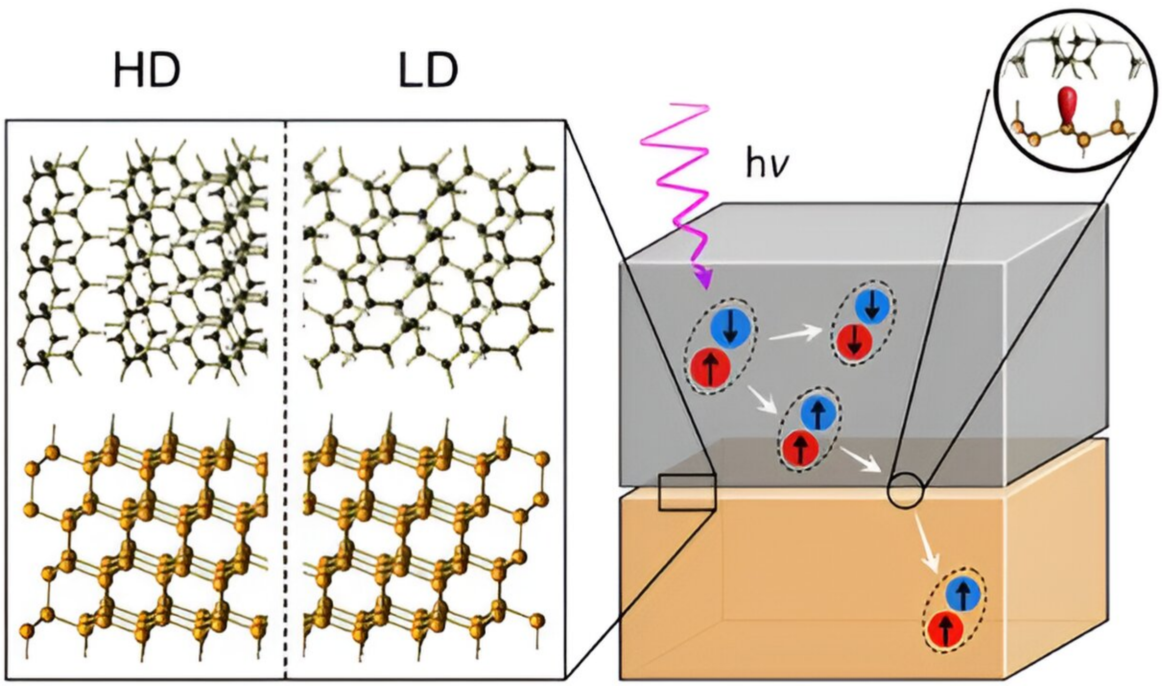
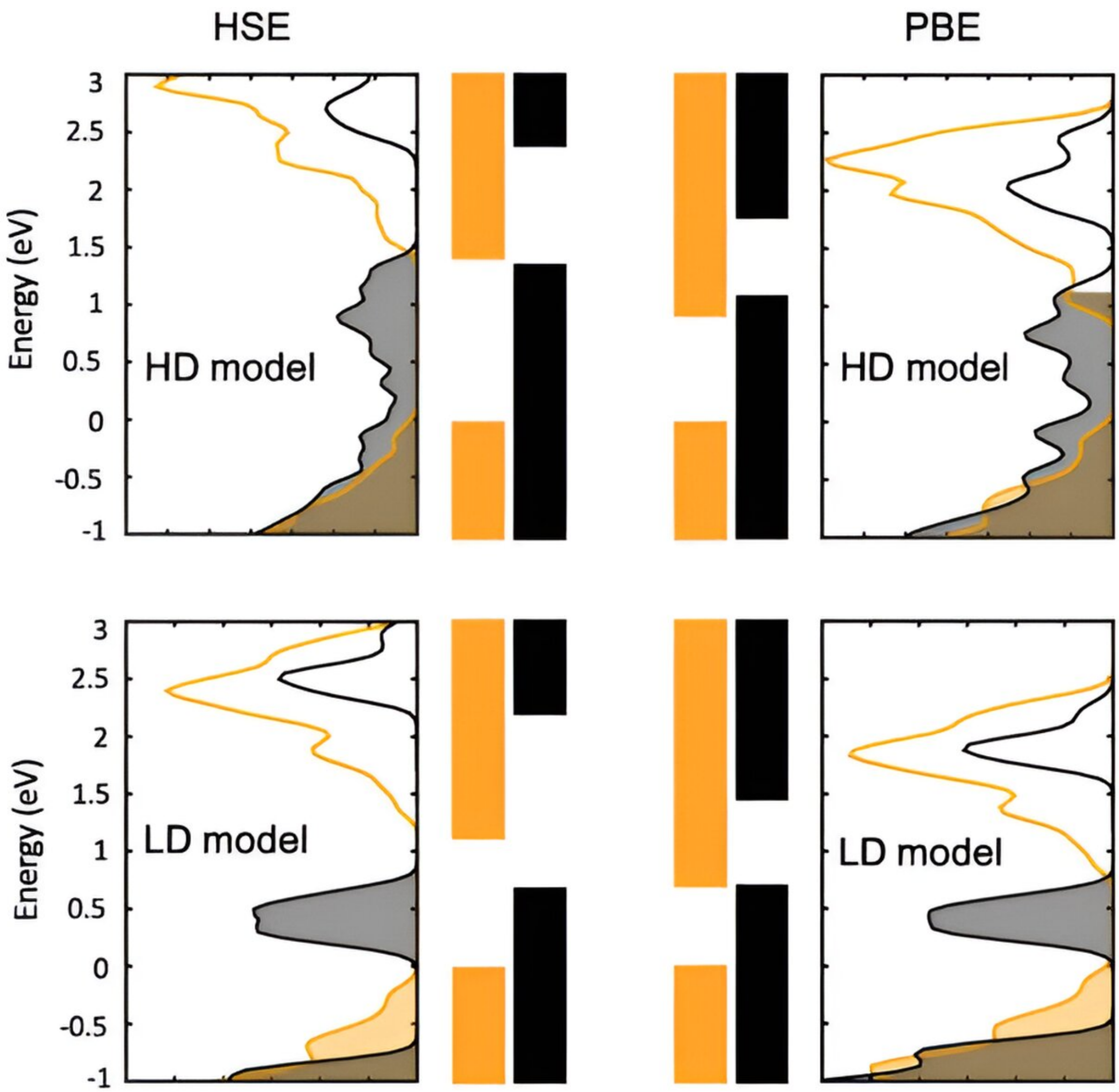


Scheme showing part of a singlet fission-sensitized silicon solar cell. Absorption of a high-energy photon by the tetracene layer produces a singlet exciton. This singlet exciton undergoes singlet fission to generate two triplet excitons. These excitons are then transferred into the Si solar cell. Enlarged image details (left) show side views of the models used for the interface between Si(111):H and high-density (HD) as well as low-density (LD) Tc phases. Also shown is an interface dangling bond defect (right). Credit: *Physical Review Letters* (2024). DOI: 10.1103/PhysRevLett.132.076201

Physicists at Paderborn University have used complex computer simulations to develop a new design for significantly more efficient solar cells than previously available. A thin layer of organic material, known as tetracene, is responsible for the increase in efficiency. The results have now been published in *Physical Review Letters.*

"The annual energy of solar radiation on Earth amounts to over one trillion kilowatt hours and thus exceeds the global energy demand by more than 5,000 times. Photovoltaics, i.e., the generation of electricity from sunlight, therefore offers a large and still largely untapped potential for the supply of clean and renewable energy. Silicon solar cells used for this purpose currently dominate the market, but have efficiency limits," explains Prof Dr. Wolf Gero Schmidt, physicist and Dean of the Faculty of Natural Sciences at Paderborn University. One reason for this is that some of the energy from short-wave radiation is not converted into electricity, but into unwanted heat.

Schmidt explains, "In order to increase the efficiency, the silicon solar cell can be provided with an organic layer, for example made from the semiconductor tetracene. Short-wave light is absorbed in this layer and converted into high-energy electronic excitations, so-called excitons. These excitons decay in the tetracene into two low-energy excitations. If these excitations can be successfully transferred to the silicon solar cell, they can be efficiently converted into electricity and increase the overall yield of usable energy."



Density of states and band alignment for Tc overlayers on Si(111):H calculated on the HSE and PBE levels of theory. Energies refer to the Si valence band maximum (VBM). Black and orange denote Tc- and Si-related states, respectively. Occupied states are shaded. Credit: *Physical Review Letters* (2024). DOI: 10.1103/PhysRevLett.132.076201

Decisive breakthrough for rapid energy transfer

The excitation transfer of tetracene into silicon is being investigated by Schmidt's team using complex computer simulations at the Paderborn Center for Parallel Computing (PC2), the university's high-performance computing center. A decisive breakthrough has now been achieved: In a joint study with Dr. Marvin Krenz and Prof. Dr. Uwe Gerstmann, both from Paderborn University, the scientists have shown that special defects in the form of unsaturated chemical bonds at the interface between the tetracene film and the solar cell dramatically accelerate the exciton transfer.

Schmidt notes, "Such defects occur during the desorption of hydrogen and cause electronic interface states with fluctuating energy. These fluctuations transport the electronic excitations from the tetracene into the silicon like a lift."

Such "defects" in solar cells are actually associated with energy losses. This makes the results of the trio of physicists all the more astonishing.

"In the case of the silicon tetracene interface, the defects are essential for the rapid energy transfer. The results of our computer simulations are truly surprising. They also provide precise indications for the design of a new type of solar cell with significantly increased efficiency," Schmidt states.

More information: Marvin Krenz et al, Defect-Assisted Exciton Transfer across the Tetracene-Si(111):H Interface, *Physical Review Letters* (2024). DOI: 10.1103/PhysRevLett.132.076201
journals.aps.org/prl/abstract/ … ysRevLett.132.076201

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