# ADVANCED FUNCTIONAL MATERIALS

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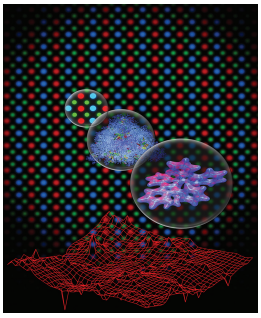
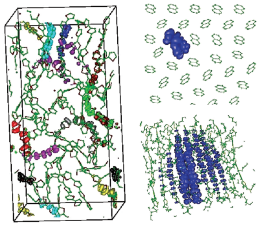


**Organic Semiconductors**

On page 1955 P. Kordt, D. Andrienko, and colleagues illustrate different approaches for modeling the charge transfer of an amorphous phase of DPBIC, a compound used in hole-conducting and electron-blocking layers in blue phosphorescent organic light-emitting diodes. In particular, it is shown how material properties such as density, radial distribution functions, ionization potentials and electron affinities, energetic disorder, charge mobility, and current–voltage characteristics can be extracted from simulations.

**Charge Mobility**

Organic semiconductor materials exhibit different types of disorder, which lead to the localization of charge carrier wave functions. On page 1915, M. Mladenović and N. Vukmirović show that atomic multiscale simulations can be used to generate the models of atomic structure and to calculate the wave function localization lengths, electronic density of states, and sometimes even the conductivity of the material.

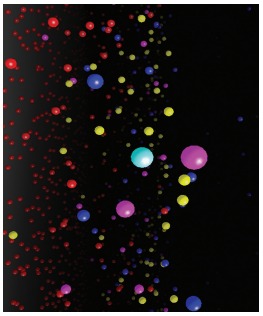



**Charge Transport**

The effects of charge delocalization on device efficiency are probed by G. R. Hutchinson and co-workers using mesoscale Monte Carlo simulations of charge transport in idealized and isotropic two-phase morphologies. As shown on page 1996, interfacial charge trapping is drastically reduced when Coulomb interactions are weakened through moderate delocalization (1.0–2.0 nm). Morphological differences become less dominant as charges delocalize.

**Optoelectronics**

Kinetic Monte Carlo simulations are used by R. Coehoorn and team on page 2024 to mechanistically analyze the influence of organic semiconductor materials properties on the luminance decay due to degradation processes in phosphorescent organic light-emitting diodes. A relationship is established between the lifetime and the efficiency roll-off with increasing current density, assuming triplet-polaron quenching processes as the root-cause of the degradation, and design rules regarding the energy levels are developed.

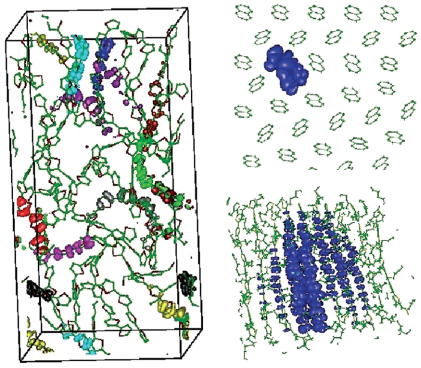


## EDITORIAL



## FEATURE ARTICLES

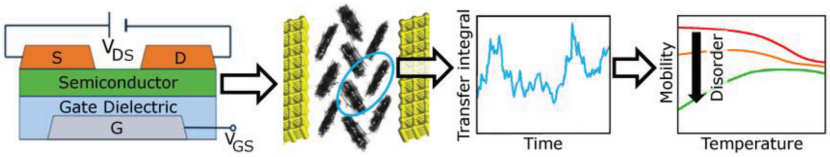
**Organic semiconductor materials** exhibit different types of disorder which lead to the localization of charge carrier wave functions. Atomic multiscale simulations can be used to generate the models of atomic structure and to calculate the wave function localization lengths, electronic density of states, and sometimes even the conductivity of the material.



### Charge Mobility



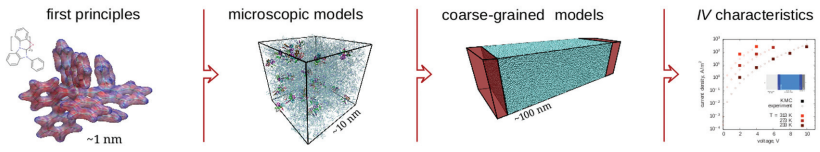
**Molecular semiconductors** are intriguing materials with applications in flexible electronics due to their potential low-cost processing ability and chemical tunability. In addition, they are utile in fundamental studies of decoherence effects in single-molecular junctions. Concepts of transport modeling for such systems are presented in this Feature Article, highlighting the unique transport properties of organic and molecular semiconductors.




### Organic Semiconductors



**Multiscale ansatz for modeling of organic light emitting diodes (OLEDs)**: Single-molecule-based first principle calculations, parameterization of microscopic and coarse-grained models, simulation of *IV* characteristics are discussed. OLED properties can be predicted without fitting parameters, starting from chemical structures of compounds.




### Organic Electronics

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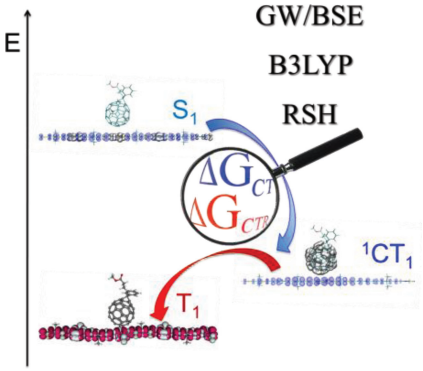
## Charge Transfer

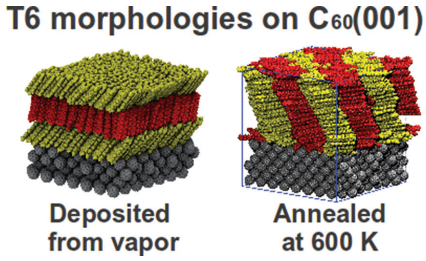





**A comparative first-principle study** is presented of polymer-fullerene complexes that differ by the excess energy for charge separation. The measured quantum efficiencies of the bulk heterojunctions can be traced back to the presence of energy-accessible charge-transfer states with large electron-hole radii and molecular triplets mediating competing recombination pathways.

## Solar Cells



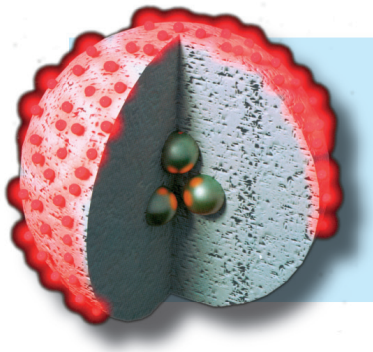



**The morphology of sexithiophene thin films** deposited over a C60 fullerene crystalline slab is investigated with an atomistic molecular dynamics technique. Simulations show that the nucleation and growth of vapor-deposited sexithiophene leads to the formation of weakly correlated crystalline layers of standing molecules, while the orientation of sexithiophene molecules can be radically changed to planar upon thermal annealing.

## Charge Transport




**The effects of charge delocalization on device efficiency** is probed using mesoscale Monte Carlo simulations of charge transport in idealized and isotropic two-phase morphologies. Interfacial charge trapping is drastically reduced when Coulomb interactions are weakened through moderate delocalization (1.0–2.0 nm). Morphological differences become less dominant as charges delocalize.

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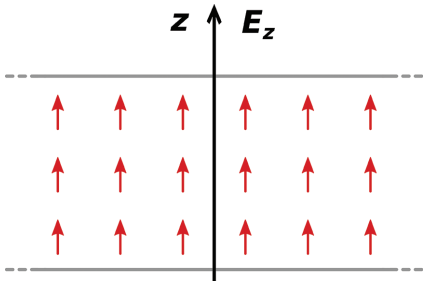
## FULL PAPERS

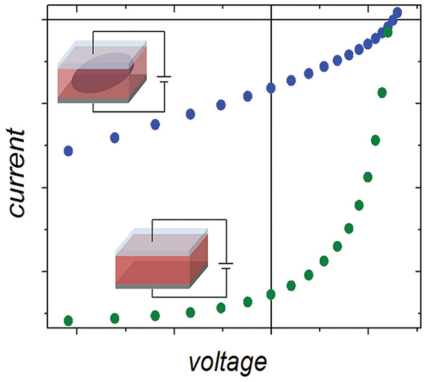
**The relative permittivity $\kappa = \varepsilon/\varepsilon_0$ of crystalline thin films** is obtained in the limit of zero intermolecular overlap. Dipole-field sums over polarizable points in applied field $E$ are evaluated directly and combined with Lorentz factors to compute $\kappa$ from monolayers to crystals, deviations from uniform polarization in surface layers, and dielectric properties in systems of lower than cubic symmetry.




### Thin Films



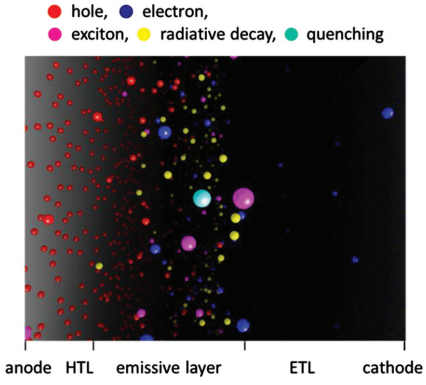
**A three-dimensional model** is presented to relate the efficiency of bulk heterojunction solar cells to the morphology of the active layer. With this, the effect of the occurrence of large acceptor domains dispersed in a mixed phase is quantified. The total current is split up in two contributions, both of which are calculated also with a one-dimensional drift–diffusion model.




### Organic Electronics



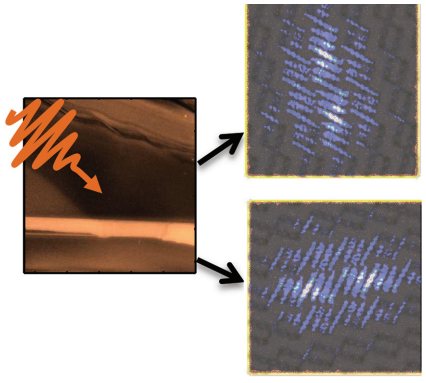
**Kinetic Monte Carlo simulations** are used to mechanistically analyze the influence of organic semiconductor materials properties on the luminance decay due to degradation processes in phosphorescent organic light emitting diodes. A relationship is established between the lifetime and the efficiency roll-off with increasing current density, assuming triplet-polaron quenching processes as the root-cause of the degradation, and design rules regarding the energy levels are developed.




### Optoelectronics



**A combination of micro-spectroscopy and many-body perturbation theory** reveals the inter-grain orientation within polycrystalline TIPS-pentacene films and the relationship of the physical structure to optoelectronic properties.

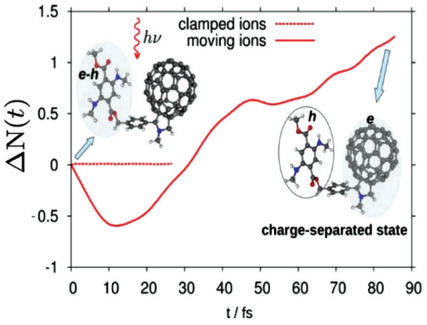


### Organic Semiconductors

## FULL PAPER

### Charge Separation






**Photoinduced charge separation** occurs on a 100 fs time scale in a diaminoterephthalate-$C_{60}$ dyad. Quantum simulations are performed to study the excited state dynamics of a new dyad. The chemical flexibility and optical properties of the chromophore moiety make this system a particularly useful model to study the early steps in the photovoltaic energy conversion. The simulations clarify the influence of electron-nuclei coupling and molecular conformation on the charge separation efficiency of the molecule.

## HIGHLIGHT

### Van der Waals Interactions




**Van der Waals interactions** arise from correlated electronic fluctuations in matter and are therefore present in all materials. Current understanding of these ubiquitous quantum-mechanical forces is summarized, and their effects in a wide variety of realistic materials are highlighted, ranging from molecular assemblies to solids with and without defects, nanostructures of varying size and dimensionality, as well as interfaces between inorganic and organic materials.