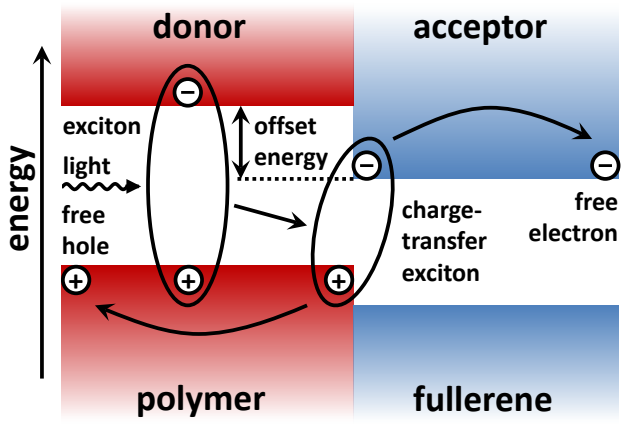
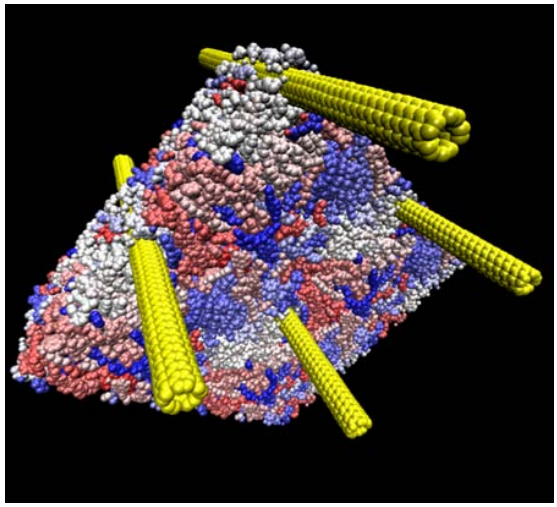
Charge separation in organic solar cells

Organic solar cells consist of a mixture of an electron-donating material, often a semiconducting polymer, and an electron-accepting material, often C_{60} (Buckminster fullerene). Charge separation in these solar cells has been identified as the crucial factor determining their efficiency. The process is critically dependent on the morphology of the donor-acceptor interface at the atomic scale. Both an intimate contact between donor and acceptor is required for fast charge transfer across the junction, as well as a sufficient amount of crystallinity of either or both components to facilitate long-range charge separation. In this project atomistic molecular-dynamics (MD) simulations will be combined with electronic-structure (ES) calculations to investigate charge separation in these solar cells and to establish the optimal conditions for this process. The project will be jointly supervised by Alexey Lyulin (MD simulations) and Peter Bobbert (ES calculations).



In this proposal the critical step in organic bulk-heterojunction solar cells will be investigated: the separation into free charges of charge-transfer excitons, created at the polymer-fullerene interface from diffusing optically generated excitons in the polymer.



Snapshot of an atomistic MD simulation of a polyimide-carbon nanotube composite. In this project such simulations will be performed for polymer-fullerene interfaces to investigate the atomistic morphology and its influence on charge separation.