



Quantum Efficiency Seminar und Colloquium

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Simulation of the laser induced fluorescence (LIF) spectrum of the conjugated polymer PTCDA

Conjugated polymers such as 3,4,9,10-perylenetetracarboxylic dianhydride (PTCDA) are materials of great interest since they can be used as active semiconductors in optoelectronic devices e.g. light emitting diodes or organic solar cells. In optoelectronic devices these polymers are part of molecular the donor-acceptor complexes which form the active layer for the conversion of light into electric current and vice versa. As a part of the conversion charge transfer from the donor to the acceptor molecule takes place, a process that is not fully understood. It is particularly difficult to decide which parameters, like structure, conformation and distance between donor and acceptor significantly influence the charge transfer process. Charge transfer complexes will be investigated in the near future with high precision optical methods like LIF at ultralow temperatures in helium nanodroplets and characterized with the help of accompanying simulations. As a starting point we show that the simulated LIF spectrum of PTCDA matches favourably the measured spectra. This study enables to learn about the required accuracy level in our ab initio calculations. I also present the application of the method to zinc phthalocyanine (ZnPc), a widely used electron donor material in organic solar cells

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