

Abstract Submitted
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Photo-induced modulation in the dipole moment of a donor-acceptor pair of organic molecules¹ YOSHIYUKI MIYAMOTO, National Institute of Advanced Industrial Science and Technology, Japan, MINA YOON, ORNL, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft — We have investigated the photo-induced electron dynamics in donor-acceptor pairs of organic molecules. Specifically we will discuss TTF and TCNQ molecules and study their electron dynamics under illumination by means of time-dependent density functional theory within the local-density approximation. In their stable molecular structure, we find that these molecules align in parallel and show maximum optical oscillator strength with an optical polarization parallel to their molecular axis. Without illumination, a dipole moment from TTF to TCNQ directs perpendicular to the molecular axis. This dipole-moment is further increased upon illumination with an optical polarization parallel to the molecular axis at resonant excitation energies of 2.00 eV and 3.55 eV. The light-induced increase of the dipole moment, which reflects the separation of electron and hole pair, is caused by the internal electric field between these molecules. Therefore, these molecules may have a high potential as building blocks of future organic photovoltaic devices.

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