Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Theoretical design of near - infrared organic compounds. KATARZYNA BRYMORA, LAURENT DUCASSE, University of Bordeaux, OLIVIER DAUTEL, Universit Montpellier 2, CHRISTINE LARTIGAU-DAGRON, Universit de Pau et des Pays de l'Adour, FRDRIC CASTET, University of Bordeaux — The world follows the path of digital development faster than ever before. In consequence, the Human Machine Interfaces (HMI) market is growing as well and it requires some innovations. The goal of our work is to achieve an organic Infra-Red (IR) photodetectors hitting the performance requirements for HMI applications. The quantum chemical calculations are used to guide the synthesis and technology development. In this work, in the framework of density functional theory (DFT) and time-dependent density functional theory (TD-DFT), we consider a large variety of materials exploring small donor-acceptor-donor molecules and copolymers alternating donor and acceptor monomers. We provide a structure-property relationship in view of designing new Near-Infrared (NIR) absorbing organic molecules and polymers.

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Date submitted: 12 Nov 2016 Electronic form version 1.4