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Theoretical modelling of high-dielectric constant donors for high-conversion organic film solar cells KENJI MISHIMA, KOICHI YAMASHITA, The University of Tokyo, JST-CREST — In this contribution, we report our theoretical design of high dielectric-constant donors based on the DFT and TD-DFT quantum chemistry calculations. The motivation of our study lies in the importance of high-dielectric constant donors and acceptors for purposes of separating photo-generated excitons efficiently and preventing them from recombining, thus leading to high photo-conversion efficiency in the organic film solar cells. Our theoretical design guideline is to bind the conventional thiophene-related one-dimensional donor molecules via benzene rings two-dimensionally, which leads to extended pi-conjugation and their high dielectric constants. Our numerical results indicate that the dielectric constant increases monotonically with the size of the molecule. The dielectric constant of the two-dimensionally extended thiophene donor amounts to 13.6, which is more than three times as much as that of the conventional P3HT donor molecule (~ 4). By using PCBM molecule as an acceptor, the total amount of photo-induced transferred charge transfer from the donor to the acceptor is comparable to that of the P3HT/PCBM system.

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