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**Understanding the charge-transfer phenomena between prototypical electron-donors and acceptors: TTF-TCNQ as an example**
CHANGWON PARK, Center for Nanophase Materials Science, Oak Ridge National Lab, VIKTOR ATALLA, Fritz Haber Institute of the Max Planck Society, SEAN SMITH, Oak Ridge National Lab, MINA YOON, Center for Nanophase Materials Science, Oak Ridge National Lab — It is widely accepted that the charge transfer between the conventional electron donor and acceptor molecules is independent of their relative configurations and electrons are always transferred from the molecule with the lower ionization potential, the electron-donor, to the high electron affinity molecule, the electron-acceptor. Conventional first-principles density functional theory (DFT) supports this conclusion. However, the computational results are dominated by a term in the DFT exchange-correlation functional, which often results in qualitatively and quantitatively wrong conclusion due to an artifact. In our study of prototypical electron donor-acceptor molecules, TTF-TCNQ, we show that the conventional electronic picture is not valid and the relative orientation between TTF and TCNQ is equally important as the electronic structure of the individual molecules. Our results show that the current understanding of the donor-acceptor interaction and charge transfer mechanism has to be modified. This research was conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Office of Basic Energy Sciences, U.S. Department of Energy.

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