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Material Design Inputs from Charge Density Analysis in Organic Semiconductors

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In recent years, semiconducting organic materials have attracted a considerable amount of interest to develop all-organic or hybrid organic-inorganic electronic devices such as organic light-emitting diodes (OLEDs), organic field-effect transistors (OFETs), or photovoltaic cells. Rubrene (5,6,11,12-tetraphenyltetracene, RUB) is one of the most explored compound in this area as it has nearly 100% fluorescence quantum efficiency in solution. Additionally, the OFET fabricated by vacuum-deposited using orthorhombic rubrene single crystals show p-type characteristics with high mobility up to 20cm²/Vs (Podzorov et al., 2004). The large charge-carrier mobilities measured have been attributed to the packing motif (Fig a) which provides enough spatial overlap of the π-conjugated tetracene backbone. In the same time, RUB undergoes an oxidation in the presence of light to form rubrene endoperoxide (RUB-OX) (Fumagalli et al., 2011). RUB-OX molecules show electronic and structural properties strikingly different from those of RUB, mainly due to the disruption in the conjugate stacking of tetracene moieties. The significant semiconducting property of RUB is not clear yet. In this context, high resolution single crystal X-ray data of RUB (Fig b) and RUB-OX have been collected at 100K. Owing to the presence of weak aromatic stacking and quadrupolar interactions, the neutron single crystal data is also collected at 100K. The C-H bond distances and scaled anisotropic displacement parameters (ADP) of hydrogens from the neutron experiment are used in the multipolar refinements of electron density. The chemical bonding features (Fig c), the topology of electron density and strength of weak interaction are calculated by the Atoms in Molecules (AIM) theory (Bader, 1990). It is further supported by the source function description and mapping of non-covalent interactions based on the electron density. The detailed comparison of two organic semiconductors, RUB and RUB-OX will be discussed.

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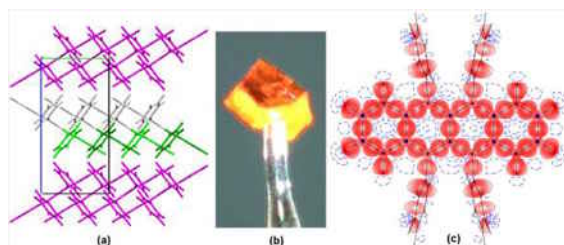
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