

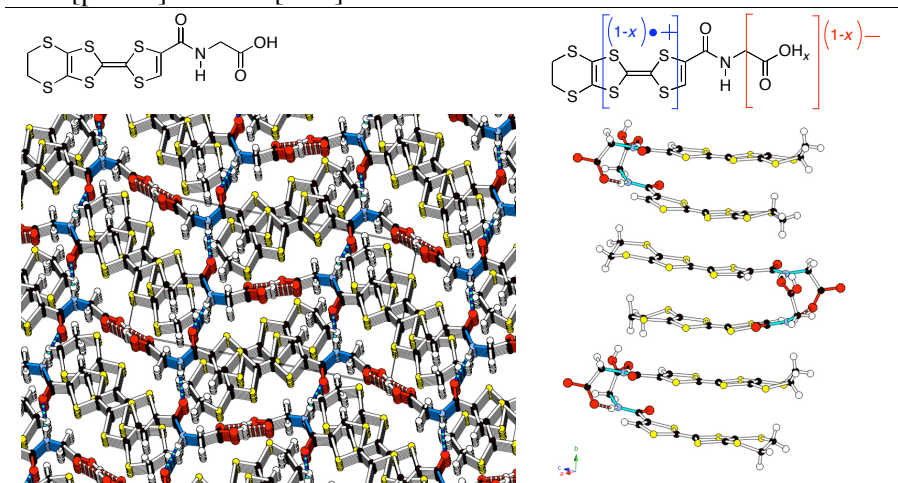
Dual [proton]/[hole] mixed-valence in molecular conductors and its relevance to charge transport in biology

Patrick Batail

CNRS-Université d'Angers / RIKEN

The dual [proton]/[hole] mixed-valence phenomenon is defined as the duality between (i) the modulation of the electrostatic potential of the environment and (ii) the incommensurate number and physics of migrating holes within a molecular system. We report on this concept as revealed in a set of case studies of (1) TTF-peptidics and their single-component, zwitterionic radicals; and (2) two-component metals based on functional radical cation salts of bi-carboxylates. These include, EDT-TTF-CO-GLY and Me₂-TTF-CO-GLY and their zwitterions^[1] (Figure 1);

Figure 1. Two monoconstituent solids which only differ by a fraction of one [proton] and one [hole]



and (EDT-TTF-I₂)₂[fumarate], (EDT-TTF-I₂)[diiodofumarate] and (EDT-TTF-CONH₂)₂[fumarate]), whose structures, phase transitions and transport properties will be discussed.

One objective here is to try and create systems whose low dimensional physics is specific of a response to the [proton]/[hole] mixed valence duality. By the same token, a change of perspective offers a way to consider and explore the effect of the pK_a values

of ionizable residues-appended redox cores on the hole migration, that is, of the modulation of the electrostatics of the environment surrounding the conducting intermolecular framework. The integration of these viewpoints provides a whole novel, conceptual, theoretical and experimental approach and is seen as perhaps especially well suited for - and relevant to - the breath of integrated research and expertise available within the Molecular Ensemble Research consortium.

This work has been carried out in collaboration with C. Mézière, L. V. Zorina, S. Simonov, A.-L. Barrès, C. Lemouchi, Y. Lahkdar, A. El-Ghayouri and M. Giffard (Angers), P. Auban-Senzier, C. Pasquier (Orsay), E. Canadell (Barcelona) and R. Kato (RIKEN)

[1] A. El-Ghayoury, C. Mézière, L. Zorina, S. Simonov, E. Canadell, B. Nafradi, L. Fórró P. Batail Dual [proton] / [hole] mixed valence : case study of a conducting zwitterionic single-component system with a ionizable amino acid residue, to be published