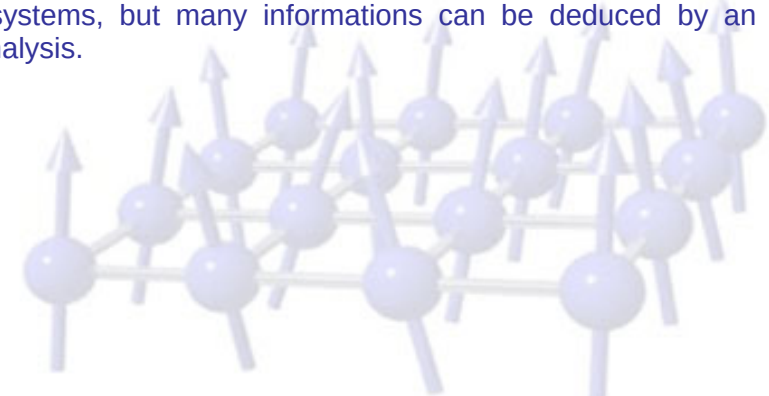
SFB/TRR 21 - Seminar
5. Februar 2008, Stuttgart

Paolo Ranzieri
(Department of Chemistry G.I.A.F., University of Parma)

Valence and structural instabilities in mixed stack organic CT crystals

Neutral-ionic phase-transition (NIT) is a fascinating phenomenon concerning many 1D mixed-stack organic crystals. These compounds show a different degree of ionicity at room temperature. Some of these are close to the neutral-ionic boundary and NIT can be induced by varying an external parameter like pressure or temperature. Temperature and pressure behavior of two mixed-stack CT crystals, the prototypical compound TTF-CA and its derivative DmTTF-CA will be discussed. They undergo both temperature and pressure induced NIT, but the interplay of electronic and structural degrees of freedom give rise to different scenarios.
Vibrational spectroscopy is a powerful tool to study this kind of structural and electronic phase transition. A complete vibrational characterization can be obtained by means of Raman and infrared single crystal investigations. Intramolecular electronic charge induces a frequency shift of many vibrational bands, and many interesting spectral features also appear due to crystal structure modifications. Electron-molecular vibration interaction also add complexity to these systems, but many informations can be deduced by an accurate vibrational analysis.



5. Februar 2008, 13:00 Uhr

Universität Stuttgart, NWZII, Raum 3.531
Pfaffenwaldring 57, 70569 Stuttgart

CO.CO.MAT