**Charge-transfer salts: Achievements**

Magnetic form factors for charge-transfer salts

- Magnetic form factor in inelastic neutron scattering:
  \[ \frac{\Delta F(q)}{F(q)} = \left( \frac{\gamma}{\Delta q^2} \right) F(q) \]

\[ F(q) = \int d^2r e^{i\mathbf{q} \cdot \mathbf{r}} \psi^*(\mathbf{r}) \psi(\mathbf{r}) \]

**Quasi-1D Fabre charge-transfer salts**

- ab initio DFT + extended Hubbard model
- Electronic properties as a function of temperature and pressure

**2D triangular spin-liquid candidates**

- ab initio-derived Hubbard parameters
- (BEDT-TTF)\(_2\)Cu\(_2\)(CN)\(_4\) :
- Me\(_2\)EtSb[Pd(dmit)]\(_2\) :
- B7 DFT + VMC
- Temperature dependence

**New donor-acceptor system TMP/HMP-TCNQ/F,TCNQ**

- Synthesis in Project B10 place
- Nature of charge transfer: combined NEXAFS B6 B12 and density functional theory calulations.

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**Project goals and program**

**Electronic effects beyond the effective dimer triangular lattice model**

Multiferroic behavior in AFM \(\kappa-(\text{BEDT-TTF})\text{Cu}(\text{CN})\text{Cl})\)

- magnetism ↔ ferroelectricity ↔ intradimer charge degrees of freedom
- \(\rightarrow\) ab initio DFT investigation + effective models
- \(\rightarrow\) dielectric response

**Neutral-Ionic transition in TTF-CA under strain**

- Polarization opposite to ionic displacement
- Ferroelectricity caused by charge transfer processes
- \(\rightarrow\) Polarization from \(\text{ab initio}\) via Wannier representation and Berry phase formalism
- \(P = P_{\text{min}} \text{ and } P_{\text{max}} = \sum_{\mathbf{k}} \int_{BZ} |\Psi(\mathbf{k})|^2 |\kappa^R_k|^2 < n_k \nabla_{\mathbf{k}} h_k >\)
- \(\rightarrow\) Strain effects on charge transfer?

**Spin liquid candidates:**

- \(\text{EtMe}_2\text{Sb[Pd(dmit)]}_{2}\)
- Anomalous uniaxial expansion
- Strong electron-lattice coupling?
- \(\kappa-(\text{BEDT-Cu}(\text{CN})_2)\)
- Anomalous thermal expansion behavior at \(T_c = \beta K\)
- Coupling of lattice, spin and charge degrees of freedom? \(\rightarrow\) \(\text{ab initio}\) molecular dynamics simulations.

**Microscopic nature of superconductivity in organic systems**

- Vicinity to Mott insulating state
- \(\rightarrow\) Hint towards spin-fluctuation-mediated SC
- Role of frustration, dimerization?
- Dimer vs. molecule description
- DFT + spin fluctuation theory + VMC