# DF 20: Focus Session: Organic ferroelectrics

Time: Thursday 9:30–12:20 Location: H11

**Invited Talk** DF 20.1 Thu 9:30 H11

**Organic Perovskites : Intriguing Magnetic Ferroelectrics** — •Naresh Dalal — Florida State University, Tallahassee, FL 32310, USAA

In an effort to synthesize lead-free perovskite ferroelectrics, we have prepared a new class of metal-organic lattices with a perovskite (ABX3) achitecture[1,2]These are compounds using early transition metals as the A-site, dimethyl amine ( or other homologues) as the B site and the O's of a carboxylic acid as the X sites. The new perovskites exhibit order-disorder as well as displacive phase transitions,with ferroelectric or antiferroelectric behaviors. They can become ferro- or antiferromagnets if magnetic ions such as Fe, Cu (II) utilize magnetic ions such as Cu(II) or Mn (II) ions or their combinations thereof . We will present polarization and NMR, specific heat and NMR relaxation data that show these materials to be glasses. The talk will present experimental as well as theoretical data showing these materials exotic ground states.

[1]Jain, Ramachandran, Clark, Zhou, Dalal, Kroto, Cheetham J. Am. Chem. Soc. 2009, 131, 13625-13627. [2]Besara, Jain, Dalal, Kuhns, Reyes, Kroto, Cheetham. Proc. Nat. Acad. Sci,, USA, 2011, 108, 6828-6832.

**Invited Talk** DF 20.2 Thu 10:10 H11

**Ferroelectricity in organic and hybrid organic-inorganic compounds** — •Alessandro Stroppa and Silvia Picozzi — CNR-SPIN Via Vetoio, 67100, L'Aquila (Italy)

Ferroelectric materials, whose spontaneous polarizations can be switched under an external electric field, have a wide range of applications in device electronics. The first ferroelectric crystal, Rochelle salt was discovered in 1920. Recent discoveries of ferroelectricity in organic solids have been limited to some well-known polymer ferroelectrics or a few low molecular mass compounds. Computational approaches based on density functional theory represent a valuable tool in order to predict or suggest new organic ferroelectrics with large values of polarization needed for device applications. In particular, the modern theory of polarization is used to estimate the ferroelectric polarization in insulating compounds and symmetry analysis gives an important help for gaining insights into the mechanisms responsible for the ferroelectric polarization. In this contribution we will focus on the description of the ferroelectric properties of organic compounds, based on density functional theory. We will focus on simple organic molecular crystals as well as complex organic-inorganic systems, such a metal-organic frameworks (MOFs). In particular, MOFs with a perovskite topology show promising new routes for the cohexistence of ferroelectricity and magnetism, i.e. multiferroicity.

**10 min. break**

**Invited Talk** DF 20.3 Thu 11:00 H11

**Coupling of charge and spin order in organic charge transfer salts** — •Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart

Organic charge-transfer salts are renown for their conducting and even superconducting properties. But the metallic phase is not stable in reduced dimensions: at low temperatures the electronic charges and spins tend to arrange themselves in an orderly fashion due to relatively strong correlations. There is a growing number of molecular materials, such as TTF-CA, TMTTF, and BEDT-TTF salts, where electronic degrees of freedom and electronic interactions are directly responsible for electric polarization and ferroelectric transition, termed electronic ferroelectricity. This would enable wide applications for organic ferroelectrics in fast switching, sensor and data storage technology.

Recently, it was discovered that charge order not only produces ferroelectricity but also breaks the symmetry of the magnetic degree of freedom in organic quantum spin chains. An intense discussion takes place whether in two-dimensional organic compounds with a high degree of frustration ferroelectric order can induce magnetic order, leading to charge-order driven multiferroicity. There are even first hints for a spin-driven multiferroic state in compounds for which the on-site Coulomb repulsion is reduced making inter-site interaction more important.

No complete picture is possible at this point, nevertheless, we have the vision that the interplay of magnetic and electronic ferroicity paves the way towards organic spintronics.

**Invited Talk** DF 20.4 Thu 11:40 H11

**Electrodynamics and ferroelectricity in two-dimensional molecular solids** — •Silvia Tomic[1], Tomislav Ivek[1,2], Marko Pinteric[1,3], Matija Culo[1], Bojana Korin-Hamzic[1], and Martin Dressel[2] — [1]Institut za fiziku, Zagreb, Croatia — [2]1.Physikalisches Institut, Universität Stuttgart, Germany — [3]Fakulteta za gradbeništvo, Univerza v Mariboru, Slovenia

A variety of organics with reduced dimensionality and competing interactions between charges, spins and lattice display a multiplicity of ordering phenomena and complex phase diagrams. Novel forms of the low-temperature phases featuring ferroelectricity in the two-dimensional molecular solids have been in the focus of intense activity in recent years. Open issues concern the nature of collective charge excitations in the charge- and spin-order-driven ferroelectric phases as well as their coupling to applied dc and ac fields. And while some of their features resemble the well-established electrodynamics of conventional charge-density waves in 1D, I will demonstrate that others appear quite different and have not been encountered until now. In the charge-ordered phase with the formation of ferroelectric domains below the metal-to-insulator phase transition, the charge response seems to be reasonably well understood within a recent theoretical model. Conversely, rather intriguing is the dielectric response in Mott insulator phases with either canted antiferromagnetism or spin liquid. The result that neither charge disproportionation nor charge fluctuations could be detected by standard experimental techniques leaves the issue of spin-charge coupling fully open.