Molecule-Based Dielectrics and Ferroelectrics

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Abstract: Molecule-based compounds bear the following advantages which are quite different from pure inorganic compound:

1. Molecule-tailor-ability in which organic molecules can be tailored according to functional purpose such as pi-pi conjugation (for fluorescent, UV-vis, NLO and thin film) and homochirality.
2. Transition-metal ion d orbit characterizations in which un-paired electrons display interesting magnetic, fluorescent and conducting properties.

The combination of above-mentioned two respects will create synergistic effect or optimization while the resulting novel multi-functional hybrid materials have widely found a lot of applications in high-technology such as laser materials (KDP) and IR detector materials (TGS) as well as FeRAM (PZT). Our investigations on molecule-based dielectrics and ferroelectrics are to mimic the above-mentioned typical compounds through crystal engineering strategy [1] and Landau theory.[2]

A Homochiral Metal-Organic Coordination type: Cobalt(II) (*R*)-2-methylpiperazine (MPPA) trichloride [Co(II)Cl_3(H-MPPA)] (**1**), was constructed through hydrogen bonds. It may be a good ferroelectric candidate with a P_s = 6.8μC·cm^{-2} high as almost twice as that of TGS (Ps=3.5μC·cm^{-2}) and significantly larger than that of KDP (5.0μC·cm^{-2}) at low temperature ferroelectric phase.[3]

Figure 1(left) Asymmetric unit perspective view of 1;(right) Its electric hysteresis loop.

B. Heterochiral Metal-Organic Coordination type: the reaction of racemic 3-methyl-piperidine (3-MePi) and pentachloroantimony (V) ($SbCl_5$) in the presence of excess concentrated HCl results in the formation of (H-3-MePi)$_2$($SbCl_7$) (**2**) which crystallizes in centric space group (*C*2/*c*) which its high temperature phase crystallizes in acentric (ferroelectric active) space group (*Ccc*2). The combination of crystal engineering strategy and Landau phase transition theory provides a powerful tool to design the polar structure at low or high temperature range if room temperature failed to.

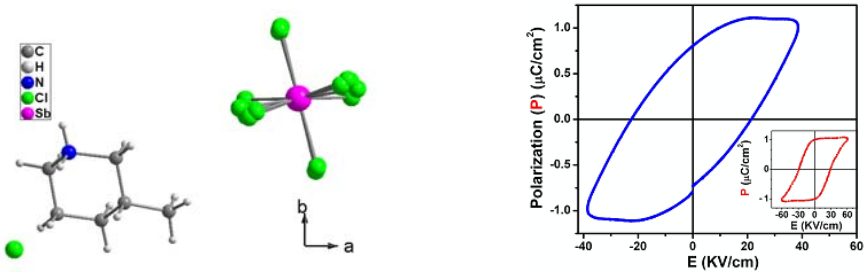

Figure 2 (left) Asymmetric unit perspective view of **2** ; (right) Its electric hysteresis loop.

References:

1. Hong Zhao, Zhi-Rong Qu, Heng-Yun, Ye, Ren-Gen Xiong, *Chem. Soc. Rev.* **2008**, *38*, 84.
2. Wen Zhang, Heng-Yun Ye, Ren-Gen Xiong, *Coord. Chem. Rev.* **2009**, in press.
3. Heng-Yun Ye, Da-Wei Fu, Yi Zhang, Ren-Gen Xiong, Songping Huang, *J. Am. Chem. Soc.* **2009,***131*, 42.