Interplay between Charge Order, Ferroelectricity, and Ferroelasticity: Tungsten Bronze Structures as a Playground for Multiferroicity

Kunihiko Yamauchi and Silvia Picozzi
CNR-SPIN L'Aquila, Italy

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Charge order is proposed as a driving force behind ferroelectricity in iron fluoride $K_{0.6}Fe_{0.6}^{II}Fe_{0.4}^{III}F_3$. By means of density functional theory, we propose several noncentrosymmetric d5/d6 charge-ordering patterns, each giving rise to polarization with different direction and magnitude. Accordingly, we introduce the concept of "ferroelectric anisotropy" (peculiar to improper ferroelectrics with polarization induced by electronic degrees of freedom), denoting the small energy difference between competing charge-ordered states.

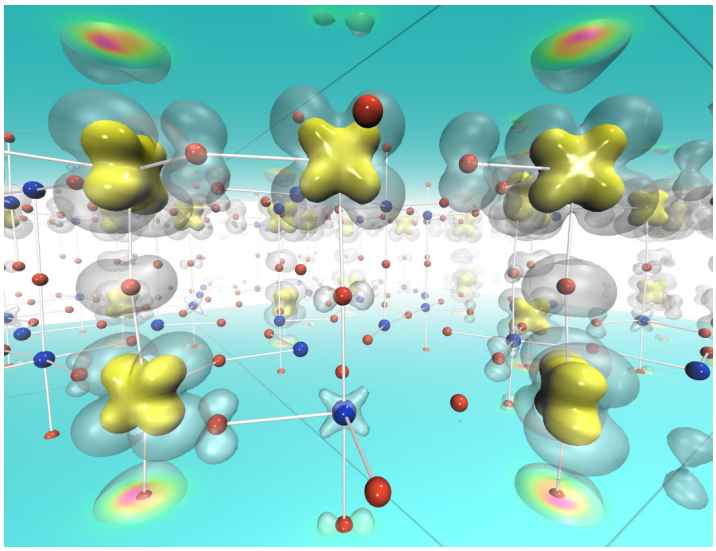

Fig. Perspective view of charge-orbital order of t2g minority-spin states in iron-fluoride K0.6FeF3

Moreover, we suggest a novel type of charge-order-induced ferroelasticity: a monoclinic distortion is induced by a specific charge-ordering pattern, which, in turn, determines the direction of polarization. $K_{0.6}Fe_{0.6}^{II}Fe_{0.4}^{III}F_3$ therefore emerges as a prototypical compound, in which the intimately coupled electronic and structural degrees of freedom result in a peculiar multiferroicity.