

Demonstration of "electronic ferroelectricity," new principle underlying electric polarization in organic ferroelectric

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Researchers from the Institute of Materials Structure Science at KEK and RIKEN discovered a new phenomenon, "electronic ferroelectricity," through electric polarization measurements and synchrotron X-ray diffraction experiments.

Electronic ferroelectricity is a mechanism by which the magnitude and direction of electric polarization in organic ferroelectrics are determined by the dynamic motion of elements between molecules. Systems exhibiting this type of ferroelectricity show polarization response to electric fields exceeding 20 times that in the classical displacement model, where static charges shift with the displacement of ions, resulting in spontaneous polarization; therefore, the discovery of the aforementioned [phenomenon](#) is expected to drive further improvement of performance in ferroelectrics.

Ferroelectrics find applications in the fabrication of nonvolatile memories, capacitors, and sensors. One urgent issue in this regard is to develop high-performance lead- or rare-metal-free organic ferroelectric materials that are lightweight, flexible, and compatible with printing processes. The valence state of tetrathiafulvalene (TTF)-p-chloranil (CA), investigated in this study, changes dramatically with temperature, thereby leading to changes in the conductivity, optical properties, and dielectric constant; therefore, TTF-CA has been attracting considerable attention from the experimental and theoretical points of view. TTF and

CA molecules are alternately stacked in the crystal at room temperature, but cooling below 81 K results in a sudden change, i.e., neutral molecules with a valence of 0.3 on an average become ionic with a valence of 0.6, and the TTF and CA molecules undergo dimerization in their respective stacks. This phase transition results in an increase in the relative dielectric constant to a few hundred units, and ferroelectricity is suggested to result from the molecular arrangement that causes electric polarization.

The research group grew high-quality TTF-CA crystals, evaluated the P-E hysteresis properties by careful choice of the measurement conditions (including temperature and frequency) to avoid dielectric breakdown, and demonstrated the ferroelectricity. In addition, synchrotron X-ray diffraction experiments at the Photon Factory determined the absolute structure and confirm the ionic displacements in the crystal.

Displacements opposite to the direction of the electric field were observed: TTF⁺ moved toward the cathode, and CA⁻ moved toward the anode. In summary, a large spontaneous polarization in the direction opposite to that of the displacement of static charges is found. The origin of this polarization is considered to be the dynamic motion of electrons, where the ionicity of molecules forming pairs increases through a neutral-to-ionic phase transition. “Electronic ferroelectricity,” in which an electronic mechanism determines the magnitude and direction of a large [electric polarization](#), is demonstrated for the first time, and its spontaneous polarization is evaluated.

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