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Structure, design and function of pyroelectric crystals

Pyroelectricity, a phenomenon first discovered in 314 BC by the Greek philosopher Theophrastus, who noticed that a mineral, presumably tourmaline, attracts or repels ash, when exposed to a temperature change. It was not until the 17th century, that it was determined that pyroelectricity is the ability of some crystals to generate a temporary voltage which is followed by attraction of depolarization charges from the surrounding. It was generally considered, that such property is confined exclusively to the polar directions of the 10 out of 32 crystal classes. Experimental observation of pyroelectricity associated with surface polarity was thought impossible because surface polarity attracts very little depolarization charges to be detectable. During the last decade; however, improvement in instrumentation provided means to measure accurately pyroelectric currents of few pico-amperes and pyroelectric coefficients of the order of 10^{-13} C/(cm^{2}K), which is 1:10000 with respect to commercially important materials. This opens interesting opportunities to apply the pyroelectric effect as a tool for searching disorders in crystals or for acquiring structural information about near polar surfaces of non-polar crystals. One of the important advantages of the pyroelectric technique is that it allows studying a large variety of materials including rough surfaces. Mechanistic studies of the formation of mixed crystals by intentional doping or by occluded impurities had demonstrated reduction in the symmetry of the non-polar hosts by converting the latter into mixed crystals composed from polar sectors. Furthermore, the occluded guests create constrained polar-domains within the host crystals, which determine their macroscopic properties. The structure of such domains can be elucidated at the molecular level by pyroelectric measurements combined by computational techniques such as DFT (density functional theory) calculations and MD (molecular dynamics) simulations. Here are described the application of these concepts for the following examples: (1) The structure of the polar domains of the doped centrosymmetric α-glycine crystals with other α-amino acids, in concentrations less than 1%, were determined at the molecular level by pyroelectric measurements combined with theoretical calculations. (2) The riddle of the anomalous pyroelectricity from the centrosymmetric α-glycine crystals is resolved by considering the landing of large clusters, present in the supersaturated solutions, during the growth of the crystals, in keeping with the non-classical mechanisms of crystal growth. (3) The detection of enantiomeric disorder, by pyroelectricity along the non-polar directions, in the racemic crystals of D,L alanine and D,L aspartic acid, which is not detectable by the diffraction techniques. (4) Freezing experiments performed on the surfaces of $LiTaO_3$ studied in a specially designed set-up, revealed that positively charged surfaces enhance, whereas negatively charged surfaces delay freezing. Differences in the operation of the pyroelectric effect on inducing ice nucleation on hydrophilic and hydrophobic surfaces will be presented.

Biography

Meir Lahav has completed his PhD and Postdoctoral and then joined the Weizmann Institute. His scientific interests comprise solid-state and surface chemistry, stereochemistry, the properties of polar crystals and the emergence of homochirality on Earth. He shared with Prof. L. Leiserowitz the Prelog Medal for Stereochemistry from ETH, the G. Aminoff Prize for Crystallography from the Swedish Academy of Science and the Israel Prize.

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