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Orientational disorder of dipolar molecules: A key to understand polarity formation in materials

Dipolar molecules (low molecular weight up to macromolecular) entering solid matter by a mechanism of growth can produce macroscopic effects of polarity. Here, we will review theoretical and experimental results on a stochastic mechanism leading to polarity in molecular crystals, inorganic-organic biomimetic materials and natural tissues. Monte Carlo model and molecular dynamics simulations support a so called bi-polar state in all these cases. The bi-polar state is characterized by two adjacent polar domains of opposite orientation of the polarization. Experimentally, the spatial distribution of polarity in materials was investigated by scanning pyroelectric (SPEM) and phase sensitive second harmonic generation microscopy (PS-SHG). These two advanced techniques allowed us for the first time to demonstrate the theoretically predicted reversal transition in molecular crystals nucleating into a polar structure, developing then two adjacent domains of opposite polarization. Similarly, PS-SHGM was applied to a first determination of the absolute polarity distribution in teeth cementum. Theoretical and experimental works on various materials allow us to conclude, that in general a bi-polar state represents the statistical ground state of materials made of dipolar constituents.

Biography

Jürg Hulliger studied physical chemistry at ETH Zürich and received a PhD from the University of Zürich. Later he moved to the Department of Physics at ETH Zürich to perform research on materials and crystal growth. Since 1993, he has been a Full Professor at the University of Berne. His research interests cover materials synthesis, physical properties and theory of condensed matter. Since 2004 he has been a fellow of the Royal Society of Chemistry. The present topic is represented by about 80 peer reviewed papers.

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