Keynote Lecture

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Stochastic polarit formation: Molecular crystals, composite materials and natural tissues

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Stochastic polarity formation in molecular crystals, composite materials and natural tissues

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By this topical review we summarize theoretical and experimental findings obtained during the last 20 years on the subject of growth induced polarity formation driven by a Markov chain process [1]. When entering a growing surface of a molecular crystal [2], an inorganic-organic composite [3] or a natural tissue [4], building blocks may undergo 180° orientational disorder. Driven by configurational entropy, faulted orientations can promote the conversion of a growing non-polar seed into an object showing polar domains. Similarly, orientational disorder at the interface may change a polar seed into a two domain state [2,5]. Analytical theory and Monte Carlo simulations were used to model polarity formation [6]. Scanning pyroelectric [7], piezoresponse force [7] and phase sensitive second harmonic [8] microscopy are methods to investigate spatial distributions of polarity. Summarizing results on different types of materials we are about to provide a general principle for obtaining growth induced polar domains for various materials: (i) A non-zero difference in the probabilities for 180° orientational misalignments of building blocks and (ii) uni-directional growth along with (iii) Markov chain theory can produce objects showing polar domains.
However, the lecture at first will address new results for three unresolved issues of polar molecular crystals in general: (i) Polar materials show charged faces undergoing compensation at ambient conditions. Here, we present calculations showing the charge distribution on faces and experimental means to investigate the net dipole moment of a crystal object. (ii) New calculations on the inner and outer electrical field of polar crystals have revealed a pronounced shape effect: Comparing needles vs plates, the direction and strength of the inner field can change and so its influence on molecular based properties. Compensation charges alter the inner and outer field. (iii) Polar crystals typically show growth anisotropy along their polar axis. Here, we discuss contradictory results for three types of crystals along with a proposition to resolve the problem.

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