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Abstract

Symmetry Breaking and Polarity Formation in Molecular Crystals †

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Dipolar molecules restricted to one single degree of freedom (180° orientation disorder) can produce growth-induced polar order in particular sectors of molecular crystals. The phenomenon can theoretically be described by an Ising model with a free boundary surface perpendicular to the growth direction. In fact, the model Hamiltonian contains a linear coupling of the spin variable of surface molecules and the elementary microscopic two-body energy. Such coupling is formally equivalent to an effective electrical field acting on those spins, breaking in this way the intrinsic spin flip symmetry [1]. This description applies to nm-sized seed crystals as well as to crystals growing to macroscopic size. In the first case, the system at equilibrium consists of a bi-polar state of general ∞∞ m symmetry. In the case of growth, a polar seed undergoes a reversal transition which also transforms the mono-domain state into a bi-polar one [2].

Phenomena to be reported represent a general behavior of condensed molecular matter formed by asymmetrical but not necessarily chiral building blocks, which split into a bi-polar state featuring zero net polarity. This is in agreement with a general statistical mechanical statement that a system in a stationary state does not show an electrical dipole moment [3].

References

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