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Information-based measures of structural complexity of crystals

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Estimating complexity of complex systems in quantitative terms is an emerging topic of research in various areas of science, including cosmology, biology, sociology, etc. In crystallography, this problem was under consideration since Linus Pauling's fifth rule of parsimony that states that 'the number of different types of constituents in a crystal tends to be small'. It was always understood that complexity is related to information: less complex systems possess less information. On the other hand, structural complexity expressed as information contributes negatively to configurational entropy. Since crystal structures can be described by a finite amount of information (space group and the number and ratio of atom sites), their information content can easily be expressed using Shannon-information measures [1]. Moreover, it can be shown that Shannon information per atom represents a negative contribution to configurational entropy of crystals [2]. This relation is also exemplified by the decrease of structural complexity across phase transitions induced by increasing temperature (associated with increasing entropy), though some exceptions are known. It is noteworthy that Shannon-information measures of structural complexity can be used for both 'classical' and aperiodic crystals, if the latter are represented as ideal crystals in n-dimensional space.

In 1662, Pierre de Fermat formulated his principle of least action, which was generalized by Pierre Louis Maupertuis, who pointed out that "Nature is thrifty in all its actions". The formation of crystals can be seen as a manifestation of this principle from the information-theoretic point of view, since symmetry may be considered as a way the Nature uses to minimize information. This is also true with regard to metastable crystallization of polymorphs in inorganic systems: in Ostwald cascades of phases, the first metastable phase is usually less complex than its stable counterpart [3]. However, the exact crystallization pathway may be influenced by other factors such as inheritance of structural elements of precursor phases, heterogeneous nucleation, etc. Neverthless, there are many examples, e.g. in geological systems, when simple polymorphs crystallize metastably instead of stable complex polymorphs. In this case, the appearance of metastable phases in rocks serves as an indicator of specific crystallization conditions.

In general, quantification of structural complexity in terms of Shannon information allows for theoretical estimation of configurational entropy of crystals that can be used to understand its role in evolution of various natural and synthetic systems involving formation and transformation of crystalline phases.

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