On group-theoretical aspects of crystal chemistry of inorganic materials

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The main goal of the presentation is to give a purely geometric view of the simulation of materials and their characteristics regardless of the specificity of the material. In particular, we consider how aspects of geometrization can be translated and implemented in materials theory. Modeling the crystallization of a multicomponent chemical system with interacting species, we assume that the generation of periodic structure occurs by breaking the spatial isotropy of the original (generic) configuration space. The idea is to effectively use the concept of structural sparsity, what may allow to reduce the symmetry group to crystallographic groups. Condensation is then seen as a consistent transition to a discrete point system characterized by the emergence of order, i.e. a certain structural organization. In the context of the closest approximation of sphere geometry, such a transition suggests an isoperimetric scheme. This scheme constructively considers atoms not as objects periodically ordered in discrete points of 3-dimensional space, but as a set of point elements with geometry that imposes octahedral symmetry constraints. To characterize the structural evolution, we focus on the corresponding manipulations of symmetry operations and on the effects caused by permutations. The symmetry change leads to discrete transformations of crystal symmetry described by the Bärnighausen tree of canonical group-subgroup relations. Discrete optimization using quantum-chemical modeling or density functional theory modeling can be performed to find the most stable and energetically favorable structural configurations among potentially possible candidate models.