GI-MS48-P10 | Mathematical justifications for crystal systems, Bravais lattices and a new continuous classification

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A crystal structure is a periodic arrangement of atoms or molecules in an infinite lattice defined by a linear basis. Crystallography distinguishes crystal systems and Bravais types of lattices. These discrete classes are justified by types of transformations that keep a given lattice stable. The groups of orthogonal transformations define crystal systems (7 in dimension 3). Any lattice has the corresponding quadratic form (a symmetric positive definite matrix) that remains invariant under orthogonal transformations. The general linear group (with integer elements) acts on the space of quadratic forms. Different strata (subgroups of various sizes) that keep a given quadratic form invariant define the Bravais class of the corresponding lattice (14 in dimension 3. Since geometric positions of atoms are continuous, crystals are more naturally classified by continuous invariants stable under atomic vibrations. The talk will outline a new continuous approach that rigorously quantifies a similarity between crystals by a proper metric (a distance function) based on geometric invariants. Then different crystals with the same chemical compositions can be connected by continuous transition paths through lowest energy barriers. Such a continuous map on the space of all crystals will show which shallow minima should be merged with closely located deeper minima that represent realistic crystals.

The ultimate aim is to resolve the "embarrassment of over-prediction" when computers only generate more hypothetical crystals without accurately predicting most promising materials. Parts of this work are done in collaboration with the groups of Andrew Cooper and Matthew Rosseinsky at the Materials Innovation Factory, Liverpool.