Abstract:

Atomic systems are regularly studied as large sets of point-like particles, and so understanding how particles can be arranged in such systems is a very natural problem. However, aside from perfect crystals and ideal gases, describing this kind of "structure" in an insightful yet tractable manner can be challenging. Analysis of the configuration space of local arrangements of neighbors, with some help from the Borsuk-Ulam theorem, helps explain limitations of continuous metric approaches to this problem, and motivates the use of Voronoi cell topology. Several short examples from materials research help illustrate strengths of this approach.