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Voronoi topology for structure analysis in atomic systems

Abstract

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