

A new, efficient algorithm for measuring the “distance” between unit cells

August 7, 2021

Abstract

A persistent problem is the need to compare unit cell parameters.

- Are these cells isomorphic?
- Is this cell already known in a database?
- Has this cell already been predicted in crystal structure prediction?
- In serial crystallography, does this cell cluster near some others?
- What is the likely crystal type for this unit cell?

We present a new, simple metric, a 7-dimensional sorted vector called DC7, based on the Dirichlet cell (also known as the Voronoi cell and the Wigner-Seitz cell). The distances between lattice points in the cell are used to form a 7-dimension, sorted vector that characterizes the lattice. We will discuss our current results and compare them to previous metrics.