A fingerprint based metric for measuring similarities of crystalline structures

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Measuring similarities/dissimilarities between atomic structures is important for the exploration of potential energy landscapes. However, the cell vectors together with the coordinates of the atoms, which are generally used to describe periodic systems, are quantities not directly suitable as fingerprints to distinguish structures. Based on a characterization of the local environment of all atoms in a cell, we introduce crystal fingerprints that can be calculated easily and define configurational distances between crystalline structures that satisfy the mathematical properties of a metric. This distance between two configurations is a measure of their similarity/dissimilarity and it allows in particular to distinguish structures. The new method can be a useful tool within various energy landscape exploration schemes, such as minima hopping, random search, swarm intelligence algorithms, and high-throughput screenings.
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