Title
Mechanical stability of cubic crystalline lattices studied using a mathematical graph representation and Gaussian process regression

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Abstract
This study utilized Gaussian process regression trained on simulated physics data to make predictions of the energy of atomic configurations in a cubic crystalline lattice based on the similarity of atomic displacements quantified using the marginalized graph kernel. Force and displacement relationships for all atoms in the supercell were produced at random simulation timesteps from the system energy predictions as they were displaced in the direction of their first, second, and third nearest neighbors. Generally, atoms displayed a restorative force towards their first and third nearest neighbors, but showed instability towards their second nearest neighbors.