Finding the lowest-energy crystal structure starting from randomly selected lattice vectors and atomic positions: first-principles evolutionary study of the Au–Pd, Cd–Pt, Al–Sc, Cu–Pd, Pd–Ti, and Ir–N binary systems

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1. Introduction

3. Evolutionary procedure for predicting crystal structures

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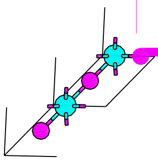

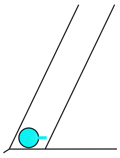

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