

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

This content has been downloaded from IOPscience. Please scroll down to see the full text.

2008 J. Phys.: Condens. Matter 20 295212

(<http://iopscience.iop.org/0953-8984/20/29/295212>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 128.138.65.115

This content was downloaded on 14/07/2015 at 17:55

Please note that [terms and conditions apply](#).

Finding the lowest-energy crystal structure starting from randomly selected lattice vectors and atomic positions: first-principles evolutionary study of the

1. Introduction

... .. '00

... ..

... .. '00

... ..

... ..

... .. \$..

... ..

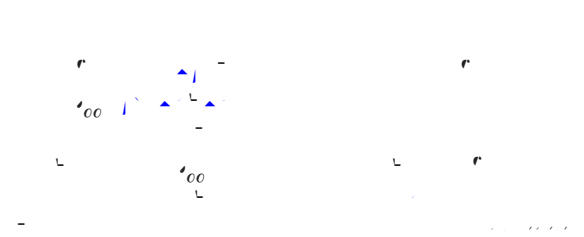
... .. \$..

... ..



3. Evolutionary procedure for predicting crystal structures

1997-2000



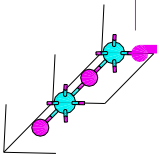
r

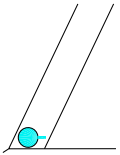
'oo

r

\$

/// / / / /
/ - / / / /
π / / / /
'oo





N_{at}

a) $(\gamma, \beta) = (1, 1)$ $(\beta, \gamma) = (1, 1)$

