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





## **3. Evolutionary procedure for predicting crystal structures**



<u>- - 20.</u> . . . . . . .

¥	L		r		-	•00	-
		,				r	
r		- r	,	\$		· · · · · · ·	·
	,		,		L		r
		Χ		/			

	/	- ,	• •
	$\pi$	111	<b>'</b> 00



N<sub>at</sub>

 $\frac{-20_{1/1}}{a} - (\gamma_{1}, \gamma_{2}) - (\gamma_$ 

- -, -