Reinterpreting the Cu-Pd phase diagram based on new ground-state predictions

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

2007 J. Phys.: Condens. Matter 19 032201

(http://iopscience.iop.org/0953-8984/19/3/032201)

View the table of contents for this issue, or go to the journal homepage for more

Download details:

IP Address: 198.11.29.40 This content was downloaded on 04/03/2017 at 16:41

Please note that terms and conditions apply.

You may also be interested in:

Bulk and surface ordering phenomena in binary metal alloys Stefan Müller

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 Giancarlo Trimarchi and Alex Zunger

Short-range-order types in binary alloys: a reflection of coherent phase stability C Wolverton, V Ozolins and Alex Zunger

Predicting the segregation profile of the Pt25Rh75(100) surface from first-principles P Welker, O Wieckhorst, T C Kerscher et al.

Configurational thermodynamics of alloys from first principles: effective cluster interactions A V Ruban and I A Abrikosov

Thermodynamic theory of epitaxial alloys: first-principles mixed-basis cluster expansion of (In, Ga)N alloy film Jefferson Zhe Liu and Alex Zunger



▼ \$, ▼ , ▼ ,



Figure 1. T > //



IOP FTC D

100

- - 19

-









Figure 5. - ζ /

 $\lfloor (l\frac{a}{a}, m\frac{a}{a}, n\frac{a}{a}) \rfloor - -$ \$ $\frac{1}{x} / \frac{1}{x} < x < \frac{1}{x} / \frac{1}{x}$ <u>،</u> ۲ L .

- - **19**, ..., ..., .

IOP

100