PCCP



CORRECTION

View Article Online
View Journal | View Issue



Cite this: Phys. Chem. Chem. Phys., 2015, 17, 28407

Correction: Study of structures and thermodynamics of CuNi nanoalloys using a new DFT-fitted atomistic potential

Emanuele Panizon, a Jimena A. Olmos-Asar, b Maria Peressi and Riccardo Ferrando*

DOI: 10.1039/c5cp90107c

www.rsc.org/pccp

Correction for 'Study of structures and thermodynamics of CuNi nanoalloys using a new DFT-fitted atomistic potential' by Emanuele Panizon et al., Phys. Chem. Chem. Phys., 2015, DOI: 10.1039/c5cp00215j.

In the published version of the article, there are a couple of errors in Table 1. The corrected version can be found below:

Table 1 Bulk values for Cu and Ni obtained with DFT simulations and parameter sets of the potential. a is the lattice parameter, E_c is the cohesive energy per atom, B is the bulk modulus and $\Delta E_{hcp-fcc}$ is the difference in binding energy per atom between hcp and fcc bulk phases

	a (Å)	$E_{\rm c}$ (eV)	B (GPa)	$\Delta E_{\text{hcp-fcc}}$ (eV)
Cu Ni	3.649 3.518	$-3.429 \\ -4.931$	138.7 206.6	0.011 0.031
	p	q	A (eV)	ξ (eV)
Cu-Cu	10.653	2.49	0.092585	1.2437
Ni-Ni	11.7	2.045	0.096444	1.6111
Cu-Ni	11.1765	2.2675	0.1046	1.4453
E _s Cu-impurity in Ni bulk			0.194 eV	
$E_{\rm s}$ Ni-impurity in	Cu duik		0.113 eV	

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

^a Physics Department, University of Genoa, Via Dodecaneso 33, 16146, Genoa, Italy

^b Department of Physics, University of Trieste, Strada Costiera 11, 34151 Trieste, Italy

^c Physics Department, University of Genoa and CNR-IMEM, Via Dodecaneso 33, 16146, Genoa, Italy. E-mail: ferrando@fisica.unige.it