



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,<sup>a</sup> Jimena A. Olmos-Asar,<sup>b</sup> Maria Peressi<sup>b</sup> and  
Riccardo Ferrando<sup>\*c</sup>

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  $\Delta E_{\text{hcp-fcc}}$  is the difference in binding energy per atom between hcp and fcc bulk phases

	$a$ (Å)	$E_c$ (eV)	$B$ (GPa)	$\Delta E_{\text{hcp-fcc}}$ (eV)
Cu	3.649	-3.429	138.7	0.011
Ni	3.518	-4.931	206.6	0.031
	$p$	$q$	$A$ (eV)	$\xi$ (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
$E_s$ Ni-impurity in Cu bulk	0.113 eV

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

<sup>a</sup> Physics Department, University of Genoa, Via Dodecaneso 33, 16146, Genoa, Italy

<sup>b</sup> Department of Physics, University of Trieste, Strada Costiera 11, 34151 Trieste, Italy

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

