

## CORRECTION

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

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 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.

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