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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)	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_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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