## **PCCP**



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

|   | a (Å)          | $E_{\rm c}$ (eV)   | B (GPa)              | $\Delta E_{ m hcp-fcc}$ (eV) |
|---|----------------|--------------------|----------------------|------------------------------|
| Cu<br>Ni  | 3.649<br>3.518 | $-3.429 \\ -4.931$ | 138.7<br>206.6       | 0.011<br>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                       |
| $E_{\rm s}$ Cu-impurity in Ni bulk $E_{\rm s}$ Ni-impurity in Cu bulk |                |                    | 0.194 eV<br>0.113 eV |                              |
| 5 F . 7   |                |                    |                      |                              |

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

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