

ADDENDUM

A 'magnetic' interatomic potential for molecular dynamics simulations.

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A ‘magnetic’ interatomic potential for molecular dynamics simulations.

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Our colleagues pointed out that the format of numerical values given in table 3 of our paper may cause confusion and lead to an error in the numerical implementation of the potential. Below we list the values given in table 3 of our original paper, this time using conventional decimal notations. These values correspond to the same choice of parameter $\rho_c = 1$.

Table 3. Optimal parameter set for case studies I and II

	Case study I	Case study II
<i>A</i>	3.527 586 256 672 234	4.100 199 340 884 814
<i>B</i>	1.642 855 167 616 477	1.565 647 547 483 517
r_n^f		f_n
3.0	0.505 568 175 375 7052	0.933 205 668 108 8162
2.866 666 666 666 670	−0.425 555 283 113 6833	−1.162 558 782 567 700
2.733 333 333 333 330	−0.562 940 810 933 9820	−0.350 202 694 924 9225
2.6	0.431 853 088 566 5762	0.428 782 083 543 0028
2.4	—	4.907 925 057 809 273
2.3	—	5.307 049 068 415 304
r_n^f		V_n
4.1	$1.753\,386\,111\,560\,4772 \times 10^{-3}$	−0.196 067 438 741 9232
3.8	−0.932 121 957 205 9338	0.368 752 593 542 2963
3.5	1.696 463 955 030 590	−1.505 333 614 924 853
3.2	0.663 847 872 510 9788	4.948 907 078 156 191
2.9	−1.914 559 267 568 704	4.894 613 262 753 399
2.6	3.193 687 184 255 540	3.468 897 724 782 442
2.4	—	−1.792 218 099 820 337
2.3	—	80.220 695 922 469 87