Corrigendum: An interaction potential to study the thermal structure evolution of a thermoelectric material: β‐Cu2Se

Sadanandam Namsani, Bhasker Gahtori, Sushil Auluck, and Jayant K Singh

It has come to our attention that there is a typo in Table 3 of our published paper [J. comput. Chem. 2017, 38, 2161-2170 ]. In the table, the first-row parameters are for Cu-Se pair and the second-row parameters are for Cu-Cu pair. The corrected Table is given below. The charges of Cu and Se atoms are +0.895(e) and -1.790(e), respectively.

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| Table 3: β-Cu2Se potential parameters obtained using the DFT based energy-volume data. |
| Morse potential | *D*(eV) | *a* (1/Å) | *r*0 (Å) | Cut-off (Å) |
| Cu-Se | 0.1517 | 1.3917 | 3.00 | 3.5 |
| Cu-Cu | 0.4370 | 3.0341 | 2.44 | 3.5 |
| Se-Se | 0.9745 | 0.6057 | 4.68 | 4.5 |