Hi， lammps developers and users,

I want to combine an EAM potential, LJ potential and Reaxff potential to describe the Cu-C system (the EAM potential for Cu-Cu interactions, the LJ potential for Cu-C interactions and the Reaxff potential for C-C interactions) using the “hybrid” method. To test the LJ potential (), a Cu-C dimer with the distance of 3.3 Å was set in a box; however, I found that in that situation the potential energy of the Cu and C atoms are not equal and the total potential energy is not equal to that value we calculated manually (shown in Table 1). I don’t know why? All the input files for the test are also sent to you as attachments, would you please help me solve these problems ? I am looking forward to your reply, thank you very much.

Table 1. The potential energy of the Cu-C dimer and the Cu, C atoms in that Cu-C dimer.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Cu (calculated with lammps) | C (calculated with lammps) | Cu-C dimer (calculated with lammps) | Cu-C dimer (calculated manually) |
| Energy (Kcal/mole) | -0.264913 | -2.5175 | -2.7823916 | -0.7437 |

