

The formula from the LAMMPS documentation
(See http://lammps.sandia.gov/doc/pair_eam.html):

$$E_i = F_\alpha \left(\sum_{j \neq i} \rho_{\alpha\beta}(r_{ij}) \right) + \frac{1}{2} \sum_{j \neq i} \phi_{\alpha\beta}(r_{ij})$$

I am confused a little with it.

I think in your notation it should be like this:

$$E_i = F_\beta \left(\sum_{i \neq j} \rho_{\alpha\beta}(r_{ij}) \right) + \frac{1}{2} \sum_{i \neq j} \phi_{\alpha\beta}(r_{ij}),$$

where β means type of i -atom, α is type of j -atom, r_{ij} is a distance between atom i and j , $\phi_{\alpha\beta}(r_{ij}) \equiv \phi_{\beta\alpha}(r_{ij})$ is a pair-wise term of potential.

The target atom is marked as β , source atom α .

For example of Fe and H, ρ_{HFe} means electron density induced by H-atom to site on Fe-atom.

In case of Fe-type of i -atom it should be used F_{Fe} , ρ_{FeFe} , ρ_{HFe} .

Am I right thinking this way?

I think so because of the provided file format:

- ◆ density function rho(r) for element I at element 1 (Nr values)
- ◆ density function rho(r) for element I at element 2
- ◆ ...
- ◆ density function rho(r) for element I at element Nelement

Thank you.