The Tersoff-1989 potential

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Brief descriptions

- This is the Tersoff-1989 potential corresponding to [Tersoff 1989].
- It only applies to systems with one or two atom types. For systems with more atom types, one needs to use the Tersoff-1988 potential.
- Even for systems with one or two atom types, the Tersoff-1989 potential is less general than the Tersoff-1988 potential, but the Tersoff-1989 potential is faster.

Potential form

- Conventions:
  - Use $i, j, k, \cdots$ for atom **indices**.
  - Use $I, J, K, \cdots$ for atom **types**.

- The **site potential** can be written as

$$U_i = \frac{1}{2} \sum_{j \neq i} f_{\mathrm{C}}(r_{ij}) \left[f_{\mathrm{R}}(r_{ij}) - b_{ij} f_{\mathrm{A}}(r_{ij}) \right].$$

- The function f_{C} is a **cutoff function**, which is 1 when $r_{ij} < R_{IJ}$ and 0 when $r_{ij} > S_{IJ}$ and takes the following form in the intermediate region:

$$f_{\mathrm{C}}(r_{ij}) = \frac{1}{2} \left[1 + \cos\left(\pi \frac{r_{ij} - R_{IJ}}{S_{IJ} - R_{IJ}} \right) \right].$$

- The **repulsive function** f_{R} and the **attractive function** f_{A} take the following forms:

$$f_{\mathrm{R}}(r) = A_{IJ} e^{-\lambda_{IJ} r_{ij}};$$

$$f_{\mathrm{A}}(r) = B_{IJ} e^{-\mu_{IJ} r_{ij}}.$$

- The **bond-order function** is

$$b_{ij} = \chi_{IJ} \left(1 + \beta_I^{n_I} \zeta_{ij}^{n_I}\right)^{-\frac{1}{2n_I}},$$

where

$$\zeta_{ij} = \sum_{k \neq i,j} f_{\rm C}(r_{ik}) g_{ijk};$$

$$g_{ijk} = 1 + \frac{c_I^2}{d_I^2} - \frac{c_I^2}{d_I^2 + (h_I - \cos\theta_{ijk})^2}.$$

Parameters

Parameter	Units
A_{IJ}	eV
B_{IJ}	eV
λ_{IJ}	A^{-1}
μ_{IJ}	A^{-1}
β_I	dimensionless
n_I	dimensionless
c_I	dimensionless
d_I	dimensionless
h_I	dimensionless
R_{IJ}	A
S_{IJ}	A
χ_{IJ}	dimensionless

Potential file format

Tersoff-1989 potential for single-element systems

- In this case, χ_{IJ} is irrelevant. The potential file reads

```
tersoff_1989 1
A B lambda mu beta n c d h R S
```

Tersoff-1989 potential for double-element systems

- In this case, there are two sets of parameters, one for each atom type. The following mixing rules are used to determine some parameters between the two atom types i and j:

$$A_{IJ} = \sqrt{A_{II} A_{JJ}};$$

$$B_{IJ} = \sqrt{B_{II} B_{JJ}};$$

$$R_{IJ} = \sqrt{R_{II} R_{JJ}};$$

$$S_{IJ} = \sqrt{S_{II} S_{JJ}};$$

$$\lambda_{IJ} = (\lambda_{II} + \lambda_{JJ})/2;$$

$$\mu_{IJ} = (\mu_{II} + \mu_{JJ})/2.$$

- Here, the parameter $\chi_{01} = \chi_{10}$ needs to be provided. $\chi_{00} = \chi_{11} = 1$ by definition.
- The potential file reads

```
tersoff_1989 2
A_0 B_0 lambda_0 mu_0 beta_0 n_0 c_0 d_0 h_0 R_0 S_0
A_1 B_1 lambda_1 mu_1 beta_1 n_1 c_1 d_1 h_1 R_1 S_1
chi_01
```

References

- [Tersoff 1989] J. Tersoff, *Modeling solid-state chemistry: Interatomic potentials for multicomponent systems* (https://doi.org/10.1103/PhysRevB.39.5566), Phys. Rev. B **39**, 5566(R) (1989).