The Tersoff-1988 potential

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Brief descriptions

- This is the Tersoff-1988 potential corresponding to [Tersoff 1988].
- It is made to mimic the Tersoff potential in LAMMPS (https://lammps.sandia.gov/doc/pair_tersoff.html).
- The Tersoff-1988 potential is more general than the Tersoff-1989 potential, but when the Tersoff-1989 potential applies, it is better to use the Tersoff-1989 potential, because it is faster.

Potential form

- The site potential can be written as

$$U_i = \frac{1}{2} \sum_{j \neq i} f_C(r_{ij}) \left[f_R(r_{ij}) - b_{ij} f_A(r_{ij}) \right].$$

- The function f_C is a cutoff function, which is 1 when $r_{ij} < R$ and 0 when $r_{ij} > S$ and takes the following form in the intermediate region:

$$f_C(r_{ij}) = \frac{1}{2} \left[1 + \cos\left(\pi \frac{r_{ij} - R}{S - R} \right) \right].$$

- The repulsive function f_R and the attractive function f_A take the following forms:

$$f_R(r) = A e^{-\lambda r_{ij}};$$

$$f_A(r) = B e^{-\mu r_{ij}}.$$

- The bond-order is

$$b_{ij} = \left(1 + \beta^n \zeta_{ij}^n \right)^{-\frac{1}{2n}},$$

where

$$\zeta_{ij} = \sum_{k \neq i,j} f_C(r_{ik}) g_{ijk} e^{\alpha (r_{ij} - r_{ik})^m};$$

$$g_{ijk} = \gamma \left(1 + \frac{c^2}{d^2} - \frac{c^2}{d^2 + (h - \cos\theta_{ijk})^2} \right).$$

Parameters

Parameter	Units
A	eV
B	eV
λ	A^{-1}
μ	A^{-1}
β	dimensionless
n	dimensionless
c	dimensionless
d	dimensionless
h	dimensionless
R	A
S	A
m	dimensionless
α	A^{-m}
γ	dimensionless

Potential file format

- We have adopted a file format similar (but not identical) to that used by LAMMPS [1].
- The potential file for a single-element system reads:

```
tersoff_1988 1
A_000 B_000 lambda_000 mu_000 beta_000 n_000 c_000 d_000 h_000 R_000 S_000 m_000 alpha_000 gamma_000
```

- The potential file for a double-element system reads:

```
tersoff_1988 2
A_000 B_000 lambda_000 mu_000 beta_000 n_000 c_000 d_000 h_000 R_000 S_000 m_000 alpha_000 gamma_000
A_001 B_001 lambda_001 mu_001 beta_001 n_001 c_001 d_001 h_001 R_001 S_001 m_001 alpha_001 gamma_001
A_010 B_010 lambda_010 mu_010 beta_010 n_010 c_010 d_010 h_010 R_010 S_010 m_010 alpha_010 gamma_010
A_011 B_011 lambda_011 mu_011 beta_011 n_011 c_011 d_011 h_011 R_011 S_011 m_011 alpha_011 gamma_011
A_100 B_100 lambda_100 mu_100 beta_100 n_100 c_100 d_100 h_100 R_100 S_100 m_100 alpha_100 gamma_100
A_101 B_101 lambda_101 mu_101 beta_101 n_101 c_101 d_101 h_101 R_101 S_101 m_101 alpha_101 gamma_101
A_110 B_110 lambda_110 mu_110 beta_110 n_110 c_110 d_110 h_110 R_110 S_110 m_110 alpha_110 gamma_110
A_111 B_111 lambda_111 mu_111 beta_111 n_111 c_111 d_111 h_111 R_111 S_111 m_111 alpha_111 gamma_111
```

- Can you guess the file format for a triple-element system?

References

- [Tersoff 1988] J. Tersoff, *New empirical approach for the structure and energy of covalent systems* (https://doi.org/10.1103/PhysRevB.37.6991), Phys. Rev. B **37**, 6991 (1988).