The Stillinger-Weber potential

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Brief descriptions

- This is the Stillinger-Weber (SW) potential corresponding to [Stillinger 1985].
- It applies to systems with one, two, or three atom types.

Potential form

The total potential energy consists of a two-body part and a three-body part. The site potential is

$$U_i = \frac{1}{2}V_2(r_{ij}) + \frac{1}{2}\sum_{j\neq i}\sum_{k\neq i,j} h_{ijk},$$

where the two-body part is

$$V_2(r_{ij}) = \epsilon A \left[B\left(\frac{\sigma}{r_{ij}}\right)^4 - 1\right] \exp\left(\frac{1}{r_{ij}/\sigma - a}\right)$$

and the three-body part is

$$h_{ijk} = \epsilon\lambda \exp\left[\frac{\gamma}{r_{ij}/\sigma - a} + \frac{\gamma}{r_{ik}/\sigma - a}\right](\cos\theta_{ijk} - h)^2.$$

Parameters

Parameter	Units
A	eV
B	dimensionless
ϵ	dimensionless
σ	A
a	dimensionless
λ	eV
γ	dimensionless
h	dimensionless

Potential file

Single-element system

- For one-element systems, the potential file reads

```
sw_1985 1
epsilon lambda A B a gamma sigma h
```

Double-element system

- For two-element systems, the two-body parameters can generally have 3 different values and the three-body parameters can generally have 8 different values. The potential file reads

```
sw_1985 2
A_00 B_00 a_00 sigma_00 gamma_00
A_01 B_01 a_01 sigma_01 gamma_01
A_11 B_11 a_11 sigma_11 gamma_11
lambda_000 cos0_000
lambda_001 cos0_001
lambda_010 cos0_010
lambda_011 cos0_011
lambda_100 cos0_100
lambda_101 cos0_101
lambda_110 cos0_110
lambda_111 cos0_111
```

- Note that we have removed the redundant parameter ϵ in the potential file here and A and λ actually stand for ϵA and $\epsilon\lambda$.

Three-element system

- If there are three atom types, the potential file reads:

```
sw_1985 3
A_00 B_00 a_00 sigma_00 gamma_00
A_01 B_01 a_01 sigma_01 gamma_01
A_02 B_02 a_02 sigma_02 gamma_02
A_10 B_10 a_10 sigma_10 gamma_10
A_11 B_11 a_11 sigma_11 gamma_11
A_12 B_12 a_12 sigma_12 gamma_12
A_20 B_20 a_20 sigma_20 gamma_20
A_21 B_21 a_21 sigma_21 gamma_21
A_22 B_22 a_22 sigma_22 gamma_22
lambda_000 cos0_000
```

```
lambda_001 cos0_001
lambda_002 cos0_002
lambda_010 cos0_010
lambda_011 cos0_011
lambda_012 cos0_012
lambda_020 cos0_020
lambda_021 cos0_021
lambda_022 cos0_022
lambda_100 cos0_100
lambda_101 cos0_101
lambda_102 cos0_102
lambda_110 cos0_110
lambda_111 cos0_111
lambda_112 cos0_112
lambda_120 cos0_120
lambda_121 cos0_121
lambda_122 cos0_122
lambda_200 cos0_200
lambda_201 cos0_201
lambda_202 cos0_202
lambda_210 cos0_210
lambda_211 cos0_211
lambda_212 cos0_212
lambda_220 cos0_220
lambda_221 cos0_221
lambda_222 cos0_222
```

- Do we need to consider more than three atom types? I don't think so. So stop here.

References

- [Stillinger 1985] Frank H. Stillinger and Thomas A. Weber, *Computer simulation of local order in condensed phases of silicon* (https://doi.org/10.1103/PhysRevB.31.5262), Phys. Rev. B **31**, 5262 (1985).