The REBO-LJ potential for Mo-S systems

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Brief descriptions

- This is the REBO-LJ potential corresponding to [Liang 2009] and [Stewart 2013].
- It only applies to Mo-S systems.

Potential form

See [Liang 2009] and [Stewart 2013].

Parameters

See [Liang 2009] and [Stewart 2013].

Potential file format

The potential file for this potential model reads

```
rebo_mos2 2
# Nothing here, because this is a special potential model and
# the parameters are thus hard coded
```

- When preparing the xyz.in file, one has to define Mo atoms as type 0 and S atoms as type 1.

References

- [Liang 2009] T. Liang, S. R. Phillpot, and S. B. Sinnott, *Parametrization of a reactive many-body potential for Mo–S systems* (https://doi.org/10.1103/PhysRevB.79.245110), Phys. Rev. B **79**, 245110 (2009).
- [Stewart 2013] J. A. Stewart and D. E. Spearot, *Atomistic simulations of nanoindentation on the basal plane of crystalline molybdenum disulfide (MoS2)* (https://doi.org/10.1088/0965-0393/21/4/045003), Modelling and Simulation in Materials Science and Engineering **21**, 045003 (2013).

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