Usage notes

Parameters obtained by an iterative simulation-based least squares fit of the simulated $g(r)$ to the experimental $g(r)$ of liquid Au at 1773 K over $r \leq 6$ Å, and validated against the bulk solid–liquid coexistence melting temperature, the bulk isobaric heat capacity, and the size dependence of the sublimation onset and melting temperature of nanoparticles (in vacuum).

Intended use: Developed for vacuum MD simuation of Au nanoparticles — sublimation onset, sublimation-driven melting, and atom ejection. The same parameter set is transferable across the high temperate solid and liquid regimes.

Functional form and parameters

The pair potential is

$$V(r) \;=\; D_0\Big[\mathrm{e}^{-2\alpha(r-r_0)} - 2\,\mathrm{e}^{-\alpha(r-r_0)}\Big], \qquad r < r_\mathrm{c},$$

truncated and shifted to zero at r_c. The parameters are as follows:

Parameter	Value	Unit
D_0	0.190	eV
α	1.661 36	1/Å
r_0	2.9032	Å
r_c	10.0	Å

Reference implementation in LAMMPS:

```
units          metal
pair_style     morse   10.0
pair_coeff     1 1  0.190  1.66136  2.9032
pair_modify    shift yes
mass           1  196.966569
```

Source: Sankhadeep Bose, Mangaiyarkarasi Rajendiran and Bruno D'Aguanno, "On the microscopic description of sublimation and sublimation-driven melting in gold nanoparticles," *Nanoscale*, 2026, Advance Article. doi:10.1039/d6nr01124a.