

# Lecture 1: The Lennard-Jones Potential

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## The Lennard-Jones Potential

The Lennard-Jones (LJ) potential is perhaps the most commonly used potential in molecular dynamics simulations. It is used to describe the attractive and repulsive forces between two atoms.

$$V_{LJ}(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right]$$

$\epsilon$  is a constant energy, while  $\sigma$  is a constant length, and they are both interaction-specific. We can remove these constants by using the dimensionless form of the potential.

$$V_{LJ}(r) = 4 \left[ \left( \frac{1}{r^*} \right)^{12} - \left( \frac{1}{r^*} \right)^6 \right]$$

## References

- Lennard-Jones Potential. (2015). In *Chemistry LibreTexts*. [http://chem.libretexts.org/Core/Physical\\_and\\_Theoretical\\_Chemistry/Physical\\_Properties\\_of\\_Matter/Atomic\\_and\\_Molecular\\_Properties/Intermolecular\\_Forces/Specific\\_Interactions/Lennard-Jones\\_Potential](http://chem.libretexts.org/Core/Physical_and_Theoretical_Chemistry/Physical_Properties_of_Matter/Atomic_and_Molecular_Properties/Intermolecular_Forces/Specific_Interactions/Lennard-Jones_Potential)
- McGaughey, A. (2016) Dimensionless LJ Potential. <https://acatar-cmu.hosted.panopto.com/Panopto/Pages/Viewer.aspx?id=f5159578-a214-4a69-8256-0570d7a76e0e>

## Dimensionless LJ

We can calculate the energy using the dimensionless form of the LJ potential for a given distance. We can see the results in Figure 1.

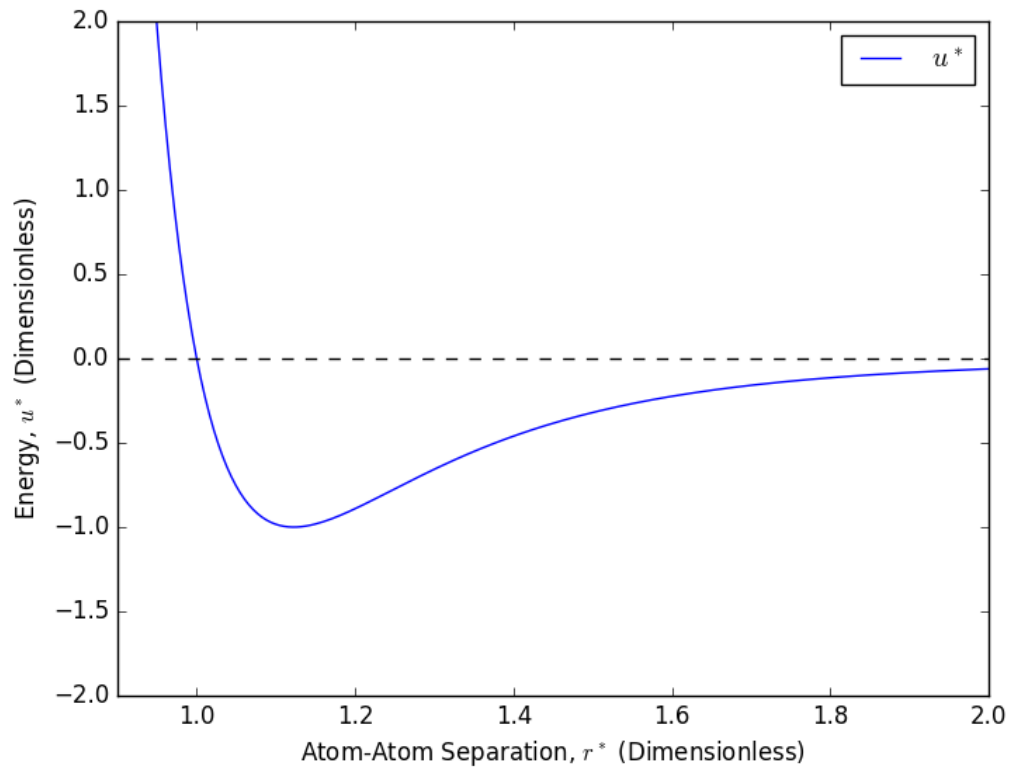


Figure 1: LJ potential for several noble gases.

## Parameters for noble gases

We can also look at the previously determined parameters and calculate the non-dimensional form of the LJ potential. Table 1 shows LJ parameters for the self-interaction of several noble gases.

Table 1: LJ parameters for noble gases.

Compound	$\epsilon/k_B$ [K]	$\sigma$ [ $10^{-12}$ m]
Ne	35.60	274.9
Ar	119.8	340.5
Kr	171.0	360.0
Xe	221.0	410.0

## References

- de With, G. (2013). Liquid-State Physical Chemistry: Fundamentals, Modeling, and Applications. Retrieved October 13, 2016, from <http://onlinelibrary.wiley.com/book/10.1002/9783527676750>

## LJ for Noble Gases

We pull the data from the previous table directly into our code and then calculate the potential for each noble gas. Figure 2 shows the potential for each gas over the specified distance range.

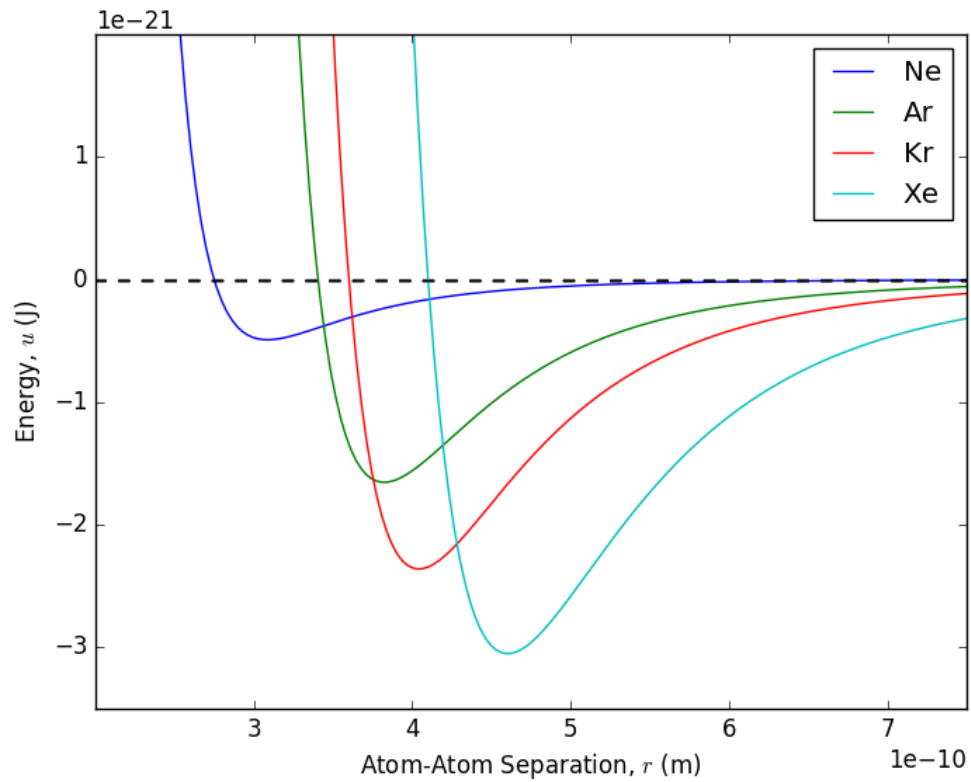


Figure 2: LJ potential for several noble gases.