# Scientific Programming with Python
# Assignment: Lennard-Jones Equation v.2

Karl N. Kirschner

Department of Computer Science, University of Applied Sciences Bonn-Rhein-Sieg,
Sankt Augustin, Germany

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**Goal** The goal of this assignment is to improve your first solution involving the Lennard-Jones equation [1], and apply it to several different situations. In doing so, you will develop a function(s), learn about built-in functions and put into practice significant figures [2, 3].

**Problem and Input Data** Computer simulations of molecular systems are often done in scientific research. The simplest atomistic model uses the Lennard-Jones potential equation to approximate how atoms are attracted and repulsed from one another [1]. The Lennard-Jones equation has the following form:

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

where $V_{LJ}(r)$ is the potential energy (in eV) of the interaction, $\epsilon$ (eV) and $\sigma$ (Å) terms are atom-dependent parameters, and $r$ (Å) is the distance between the atoms. The $6^{th}$ and $12^{th}$ powers terms model the attractive and repulsive forces, respectively.

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**Assignment Tasks**

**Task 1** Using the Lennard-Jones equation, calculate the nonbonded potential energy between two argon atoms that are separated at the following distances: 3.0, 3.4, 3.8, 4.2, 4.6 and 5.0 Å. Report all resutling energies to their significant figure (see note below), using the units Joules. For argon atoms, $\varepsilon = 0.0103$ eV and $\sigma = 3.40$ Å [4].

**Hint**: The numbers 4, 6 and 12 in the Lennard-Jones equation arise from its mathematical derivation and have infinite significant figures.

**Task 2** Identifies through code the lowest energy value and its corresponding distance from Task 1's results.

**Allowed Python3 [5, 6] functions & libraries/modules**

- All built-in functions

**Assignment Due** Turn in your solution as a **Jupyter-notebook** [7] to **LEA** by **Monday, October 30th, 2023 at 09:00**.

**Note**: Please include your **SciPro_ID** at the **top** of your notebook.

# References


[1] Wikipedia contributors, "Lennard-Jones potential." Wikimedia Foundation. Last modified August 30, 2023. https://en.wikipedia.org/wiki/Lennard-Jones_potential. Accessed on September 12, 2023.

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[3] Pacer, R. A. (2000) How Can an Instructor Best Introduce the Topic of Significant Figures to Students Unfamiliar with the Concept? Journal of Chemical Education. 77, 1435–1438. https://doi.org/10.1021/ed077p1435

[4] Rahman A. (1964) Correlations in the motion of atoms in liquid argon. Physical Review. 136(2A), A405–A411. https://doi.org/10.1103/PhysRev.136.A405.

[5] Python Software Foundation. Python Language Reference, version 3.11. Available at http://www.python.org. Accessed on October 22, 2023.

[6] van Rossum, G. Python tutorial, Technical Report CS-R9526, Centrum voor Wiskunde en Informatica (CWI), Amsterdam, 1995.

[7] Kluyver, T. et al., (2016) Jupyter Notebooks – a publishing format for reproducible computational workflows. In F. Loizides & B. Schmidt, eds. Positioning and Power in Academic Publishing: Players, Agents and Agendas. pp. 87–90.


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