Scientific Programming with Python
Assignment: Lennard-Jones Equation

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Task 1 Figure out how you want to code using Python3 (e.g. install locally, use a cloud, use an H-BRS lab).

Recommended ways for this course are:

- Jupyter Notebooks
- Google's Colaboratory
- Python via an IDE (e.g. PyCharm, Sublime)

Task 2 Write a program that reports the nonbonded interaction energy between two argon atoms that are 3.5 Å apart. Use the following 6-12 Lennard-Jones function:

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

where '$V_{LJ}(r)$' is the potential energy, 'r' is the distance between two particles (Å), 'ε' is the negative of the potential energy at the equilibrium bond length (eV), 'σ' is the separation distance where the potential energy is zero (Å).

For argon atoms, $\varepsilon = 0.0103$ eV and $\sigma = 3.40$ Å (source: Rahman, A. Phys. Rev. 1964, 136 (2A), A405–A411).

Provide the final $V_{LJ}(r)$ energy in the "International Unit for Energy."

Task 3 For fun, execute the python statement 'import this'

Turn in Task 2 to LEA by Sunday November 9th at 07:00 (morning)