Intro to Python

* Chem compute has software for comp chemists
* Jupyter notebook is IDE, type in code and immediately run code
  + lets you include text or pictures or code or equations
  + shift + enter runs

float - floating point number (decimal number)

string - word

recasting – changing data type in code

index – element in a list

for loop – do a calculation on every element in list

must click Kernel -> Restart and Run All to get code back up to date when you go back into a Jupyter notebook; if stuck, can go through a do shift+enter for individual cells after place where it got stuck