CH40208: TOPICS IN COMPUTATIONAL CHEMISTRY

PYTHONIC LOGIC AND LOOPS

LOGICAL OPERATORS

- Python and Jupiter Notebook can be used as a simple calculator
- Let's make or code more intelligent!
- To do this we can use *Boolean logic*; `True` or `False` questions
- Python is able to assess the truth of a particular operation

LOGICAL OPERATORS

DEMO

FLOW CONTROL

- We are then able to use this Boolean logic to *control* the path that the code will follow
- To do this we use `if` statements; these ask `if x is True`?
  - Note the the `is True` part is often implicit
- The `if` statement is often accompanied by an `else`; which is the path taken when `x is False`
- The third modifier in an `if` statement is the `elif` (short for else if); this offers an alternate path to follow

FLOW CONTROL

DEMO