Software Spec – Orbital Structure and OrbitalCollection Class

Atom has Orbitals corresponding to a Configuration. Atom has a Potential that is a consequence of the Orbitals.

Orbital   
 P as Double()  
 N as Integer  
 L as Integer  
 E as Double  
 Occupancy as Double

Function Sigma(

OrbitalCollection <>-- Orbital, keyed by N\_L string

Wrap a collection, expose methods to retrieve orbital based on N, L