**Quantum Dots and Quantum Yield Python**

Before running the Python script, ensure you have Psi4 installed in your Python environment. You can install Psi4 using pip

pip **install** psi4

**import** psi4  
**import** numpy **as** np  
**import** matplotlib.pyplot **as** plt  
  
# Define the molecular structure of a simple carbon quantum dot model  
**def** **create\_cqd\_structure**(num\_atoms):  
 cqd\_structure = ""  
 **for** i **in** range(num\_atoms):  
 cqd\_structure += "C 0.0 0.0 {0}\n".format(i \* 1.2) # Stacking carbon atoms vertically  
 **return** cqd\_structure  
  
# Set up Psi4 and calculate electronic properties  
**def** **calculate\_electronic\_properties**(cqd\_structure):  
 # Set Psi4 options  
 psi4.set\_output\_file('output.dat', False)  
 psi4.set\_memory('500 MB')  
  
 # Define molecule  
 mol = psi4.geometry(cqd\_structure)  
  
 # Perform Hartree-Fock calculation  
 energy, wfn = psi4.energy('SCF/6-31G(d)', return\_wfn=True)  
  
 # Get the HOMO-LUMO gap  
 homo\_energy = wfn.epsilon\_a()[0] # Highest occupied molecular orbital energy  
 lumo\_energy = wfn.epsilon\_a()[1] # Lowest unoccupied molecular orbital energy  
 gap = lumo\_energy - homo\_energy  
  
 **return** energy, gap  
  
# Plot the HOMO and LUMO energies  
**def** **plot\_homo\_lumo**(homo\_energy, lumo\_energy):  
 plt.bar(['HOMO', 'LUMO'], [homo\_energy, lumo\_energy], color=['blue', 'orange'])  
 plt.ylabel('Energy (Hartree)')  
 plt.title('HOMO and LUMO Energies of CQDs')  
 plt.show()  
  
# Main function to execute the script  
**if** \_\_name\_\_ == "\_\_main\_\_":  
 num\_atoms = 10 # Example: number of carbon atoms in the quantum dot  
 cqd\_structure = create\_cqd\_structure(num\_atoms)  
 energy, gap = calculate\_electronic\_properties(cqd\_structure)  
   
 print(f'Total Energy: {energy} Hartree')  
 print(f'HOMO-LUMO Gap: {gap} Hartree')  
   
 plot\_homo\_lumo(energy, gap)

**Explanation of the Python Script**

1. **Molecular Structure**: The create\_cqd\_structure function generates a simple carbon quantum dot structure by stacking carbon atoms in a column. This is a simplified model, and real CQDs may have complex geometries.
2. **Electronic Properties Calculation**: The calculate\_electronic\_properties function uses Psi4 to perform a Hartree-Fock calculation on the generated molecular structure. It calculates the total energy of the system and the energy gap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO).
3. **Plotting**: The plot\_homo\_lumo function visualizes the HOMO and LUMO energies using a bar chart.
4. **Execution**: The script initializes the process by creating a carbon quantum dot model with a specified number of carbon atoms, calculating its electronic properties, and plotting the results.

**Questions**

1. **Molecular Geometry**: How does the arrangement of carbon atoms in the model affect the electronic properties of the quantum dot?
2. **Energy Calculations**: What information can be inferred from the total energy calculated for the carbon quantum dot?
3. **HOMO-LUMO Gap**: Explain the significance of the HOMO-LUMO gap in determining the optical properties of carbon quantum dots.
4. **Psi4 Usage**: What are the advantages of using Psi4 for quantum chemical calculations in the context of nanomaterials research?
5. **Plot Interpretation**: Based on the plot generated for the HOMO and LUMO energies, what conclusions can you draw about the electronic structure of the synthesized carbon quantum dots?