**5. Report Sheet**

|  |  |  |  |
| --- | --- | --- | --- |
| **Name:** |  | **ID:** |  |

**Analysis 1. (20 points) Effective potential energy curve of the H2+ molecule: Ground state**

**a)** Fill out the following table using your simulation results.

|  |  |  |  |
| --- | --- | --- | --- |
| H-H distance (Å) | Total energy (Hartree) | Relative energy (Hartree) | Relative energy (**eV**) |
| 0.5 |  |  |  |
| 0.7 |  |  |  |
| 0.9 |  |  |  |
| 1.0 | -0.595799 | -0.106736 | -2.90 |
| 1.3 |  |  |  |
| 1.6 | -0.570644 | -0.081581 | -2.219933223 |
| 1.9 |  |  |  |
| 2.5 |  |  |  |
| 2.8 |  |  |  |
| 3.9 |  |  |  |
| Infinity | -0.489063 | 0.00 | 0.00 |

 - Relative energy = (Energy at given distance) - (Energy at infinite distance)

 - 1 hartree = 27.2114eV, 1 bohr = 0.529177 Å

**b)** Attach the energy-to-distance plot of the ground-state potential-energy curve of a H2+ molecule **(units in eV and bohr)**.

**Analysis 2. (20 points) Effective potential energy curve of the H2+ molecule: First excited state**

**a)** Fill out the following table using your simulation results.

|  |  |  |  |
| --- | --- | --- | --- |
| H-H distance (Å) | Total energy (Hartree) | Relative energy (Hartree) | Relative energy (**eV**) |
| 0.5 |  |  |  |
| 0.7 |  |  |  |
| 0.9 |  |  |  |
| 1.0 |  |  |  |
| 1.3 |  |  |  |
| 1.6 |  |  |  |
| 1.9 |  |  |  |
| 2.5 |  |  |  |
| 2.8 |  |  |  |
| 3.9 |  |  |  |
| Infinity | -0.489063 | 0.00 | 0.00 |

 - Relative energy = (Energy at given distance) - (Energy at infinite distance)

 - 1 hartree = 27.2114eV, 1 bohr = 0.529177 Å

**b)** Attach the energy-to-distance plot of the first excited-state potential-energy curve of a H2+ molecule **(units in eV and bohr)**.

**Analysis 3. (10 points) Visualization of orbitals**

**a)** Observe how the orbital shapes change with the H-H distance. (Use same isolevel = 0.8)

|  |  |  |
| --- | --- | --- |
| H-Hdistance(Å) | $$1σ\_{g}$$ | $$1σ\_{u}^{\*}$$ |
| 1.0 |  |  |
| 3.9 |  |  |

**b) Plot the shapes of the following orbitals at distance 1.0 Å. (Use same isolevel = 0.8)**

|  |  |
| --- | --- |
| $$1σ\_{g}$$ | $$1σ\_{u}^{\*}$$ |
| $$2σ\_{g}$$ | $$2σ\_{u}^{\*}$$ |
| $$1π\_{u}$$ | $$3σ\_{g}$$ |
| $$1π\_{g}^{\*}$$ |  |

**Analysis 4. (Optional) Attach the energy-to-distance plots of the average total Coulomb potential** $\overbar{V}$**, the average kinetic energy** $\overbar{T}$ **and the average effective potential** $\overbar{V}^{\left(eff\right)}$ **using your 10 simulations (units in eV and bohr).**

# Questions

1. Explain the degenerate state of a quantum system. State the degenerate orbitals in b) of Analysis 3. (15 points)
2. Explain the meanings of the number, σ and π, g and u, and \* in state (or orbital) symbols. In your explanation, include $1π\_{u}$, $1π\_{g}^{\*}$ and $3σ\_{g}$ orbitals of H2+ as examples. (15 points)
3. Based on your results, state the bond dissociation energy and the bond length of H2+ (no interpolation needed, roughly estimate those values). (20 points)