Calculate the electronic properties (Ionisation Potential , Electron Affinity) of Helium atom by DFT functionals using Open source software ORCA and Avogadro.

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Abstract

This works aims at predicting the electronic properties such as ionisation potential , electron affinty of Helium atom by using B3LYP DFT functionals using open source software ORCA and Avogadro. The molecule 3D geometry is build in Avogadro and through Avogadro generated ORCA input file the calculations are run on the terminal. The optimised geometry of the neutral Helium atom is used to generate the single point energy and then the unrelaxed helium cation and anion seperately is used to calculate the single point energy of these ions. Then the calculations are repeated again for the relaxed (optimised) geometry of these ions. Using the following formula the Electronic properties are calculated. Hence the theoretical calculations is observed with the experimental results.

Vertical Ionisation potential (I.P) = (Energy of He Cation unrelaxed*) - (Energy of neutral He)
Adiabatic Ionisation potential (I.P) = (Energy of He Cation relaxed*) - (Energy of neutral He)

Vertical Electron Affinity (E.A) = (Energy of neutral He) - (Energy of He anion unrelaxed*)
Adiabatic Electron Affinity (E.A) = (Energy of neutral He) - (Energy of He anion relaxed*)

Relaxed signify that the geometry of the ion is optimised while unrelaxed signify that the geometry of the ion is same as that of the neutral atom

Keyword – Orca , Avogadro, DFT, Ionisation potential, Electron Affinity