

Molecular Modeling in Process Engineering

2023/2024

Project 1

Estimation of quantized properties

The purpose is to determine the following properties as predicted from quantum chemistry theory.

- 1) Determine the zero point energy of a methane molecule in a box having the dimension of 1 m.
- 2) Determine the energy of the orbitals of atomic hydrogen, and the energy necessary for excitation between different orbitals.
- 3) Draw the 1s, 2s, 2px, 2py, and 2pz orbitals on a xy plane
- 4) Determine the average distance of an electron in a 1s, 2s, 2px, 2py, and 2pz orbital from the nuclei.