

CHEM 310 Computational Chemistry Assignment 2025

*Released 13th May and
due in at the Chemistry Office by 5pm Wednesday 28th May*

Q1 **Explain** the Coulomb and Fermi holes. **Discuss** which hole relates to the potential and which to the form of the wavefunction. **Which** is more “classical” and which is more “quantum mechanical” in nature?

(10 marks)

Q2. **Explain** $\text{Exc}[\rho]$. Write out the B3LYP functional and label the exchange and correlation parts. **Explain** the B3LYP acronym. The B3LYP functional has been effectively updated, **name** 3 of the more modern functionals, and **describe** the advanced techniques employed.

(10 marks)

Q3 **Describe** the 4-31+G(d) basis set, **explaining** each component and its purpose, **provide** an equation. **What** is the quality of this basis set, and when would it be used?

(10 marks)