

# Master 2 course in *Advanced Quantum Chemistry*

*Wavefunction theory*

$$\hat{H}\Psi = E\Psi \quad \Leftrightarrow$$

$\Psi$ : electronic wavefunction

*Density-functional theory*

$$E = F[n] + (v_{\text{ne}}|n)$$

$n$ : electronic density

- **lecturer:** *Emmanuel Fromager\**, Institute of Chemistry, Laboratoire de Chimie Quantique
- **location:** Faculty of Chemistry (Esplanade campus)

- **Content:**

In this lecture I will introduce and physically motivate the mathematical formalism underlying **electronic structure** methods that are used in standard **quantum chemical packages**.

- **Prerequisite:**

basics in **quantum mechanics** (one-electron theory) and **linear algebra** (matrix representation of operators, eigenvector, eigenvalue).

\*<https://quantique.u-strasbg.fr/doku.php?id=fr:pageperso:ef:welcome>