Lectures

The textbook for the lab: one chapter per lecture

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⬇️ Download all lectures as one PDF

Each chapter covers one lecture in more detail than there is time for in class. Read it before (or right after) the lecture. Each one ends with key points and study questions, and has a printable PDF version under *Other Formats*.

The first six lectures build the theory. Lectures 1–3 approximate the **wave function** (basis sets) and come before Experiment 1. Lectures 4–6 approximate the **Hamiltonian** (Hartree–Fock and density functional theory) and come before Experiment 2. From Lecture 7 on, each lecture looks back at the experiment you just finished and prepares the next one.

> ℹ Debrief sections
>
> From Lecture 7 on, the first part of each chapter discusses the results of the previous experiment. Read it **after** you submit that experiment. Your predictions are more useful if they're your own.

Lecture	Chapter	Comes before
1	The molecular Schrödinger equation	Experiment 1
2	Approximating the wave function: basis sets	Experiment 1
3	From theory to a calculation: IQmol, Q-Chem and Experiment 1	Experiment 1
4	Approximating the Hamiltonian I: Hartree–Fock and the SCF	Experiment 2
5	Approximating the Hamiltonian II: density functional theory	Experiment 2
6	Approximating the Hamiltonian III: Jacob's ladder	Experiment 2
7	How we test a functional	Experiment 3
8	Dispersion and noncovalent interactions	Experiment 4

Lecture	Chapter	Comes before
9	Why some reactions are hard for DFT	Experiment 5
10	Basis-set error vs functional error	Experiment 6
11	Numerical integration grids	Experiment 7
12	SCF stability, open shells and transition metals	Experiment 8
13	From electronic energies to experiment	Experiment 9
14	Choosing, running and reporting a method	Experiment 10
15	What we learned	—

For the quantum mechanics behind Lectures 1–5, see also the Live Textbook of Physical Chemistry 2.

Bibliography