Computational and Theoretical Chemistry & Physics Study Plan

Month 1: Core Math & Programming

Focus Areas:

Linear algebra, calculus, differential equations, Python, Git, Bash, LaTeX

Study Sources:

- Strang's Linear Algebra (MIT OCW)

- Boas Mathematical Methods in the Physical Sciences

- SciPy Lecture Notes

- Automate the Boring Stuff with Python

Project Ideas:

- Matrix solver in Python

- Differential equation visualizer

- LaTeX study notes

- Set up GitHub for version control

Month 2: Classical Physics & Physical Chemistry

Focus Areas:

Classical mechanics, E&M, thermodynamics, chemical bonding, kinetics

Study Sources:

- Feynman Lectures on Physics

- MIT OCW Classical Mechanics

- Atkins' Physical Chemistry

Project Ideas:

- Simulate heat conduction in Python

- Phase diagram visualizer

- Bond energy plotter for small molecules

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Month 3: Quantum Mechanics & Intro to Quantum Chemistry

Focus Areas:

Schrodinger equation, operators, orbitals, Hartree-Fock theory

Study Sources:

- Griffiths Introduction to Quantum Mechanics

- McQuarrie Quantum Chemistry

- Levine Quantum Chemistry

Project Ideas:

- Quantum particle in a box simulator

- Visualize hydrogen atom orbitals

- Run first calculations in Psi4 or ORCA

Month 4: DFT & Molecular Simulations

Focus Areas:

DFT theory, basis sets, PES, vibrations, geometry optimization

Study Sources:

- Jensen Essentials of Computational Chemistry

- Psi4 tutorials

- ORCA documentation

Project Ideas:

- DFT optimization of water and caffeine

- Calculate HOMO-LUMO gaps

- Compare DFT methods on same molecule

Month 5: Molecular Dynamics & Solid-State Physics

Focus Areas:

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MD simulations, band structures, Bloch theory, lattice dynamics

Study Sources:

- GROMACS documentation

- Quantum ESPRESSO tutorials

- Solid State Physics Ashcroft & Mermin

Project Ideas:

- Simulate water box in GROMACS

- Calculate Si band structure in QE

- Vibrational mode analysis

Month 6: Advanced Theory & Capstone

Focus Areas:

Post-HF methods, condensed matter, quantum statistics, final project

Study Sources:

- Szabo & Ostlund Modern Quantum Chemistry

- Altland & Simons Condensed Matter Field Theory

- Research papers from arXiv, JCTC

Project Ideas:

- Capstone: replicate a published study

- GitHub repository of all simulations

- Blog or PDF write-up of findings