Study Plan for Thesis

Gurjot Singh

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1 Chapter 1

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2 Chapter 2

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3 Chapter 3

3.1 Model Hamiltonian

- HDvV Hamiltonian
- Spin Hamiltonian
  - Focus on Zeeman
  - Study other stuff

3.2 EPR and g-tensor

- Read up on EPR theory
- Know what the direction vector of the g-tensor signal is.

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4 Chapter 4

- Mention how this study demonstrated that computational chemistry is about finding balance between accuray and computational cost.

4.1 BS DFT

4.2 CASSCF

- Pipek-Mezey localization scheme for double-shell orbs.

4.3 DDCI

- Know the difference between DDCI1, DDCI2 and DDCI3.
- Read about T_{sel} parameter.

4.4 BS Coupled Cluster

- Need to read on the CC ansatz and how it works.
- Know the difference between CCSD and CCSD(T).
- Read local methods and how they work.
- Difference between LPNO and DLPNO.
- Difference between all the parameters in LPNO approx: T_{CutPNO}, T_{CutPair} and the 3rd one. (see ORCA docs)

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5 Chapter 5

5.1 Experimental UV-Vis

- Read up on UV-Vis spectroscopy.
- Beer-Lambert law.
- intermediate **1** and **2** were in equillibrium at 233 Kelvin. Read up how equillibrium const are calculated.

5.2 Experimental EPR

- You know epr well enough, especially for g-tensors.
- Difference between frozen and solution based EPR spectra.
- Read up on hyperfine coupling constants.
- hyperfine coupling change with lewis acid.

5.3 XANES and TD-DFT

- Read up on XANES/X-ray spectroscopy.
- TD-DFT, know a little bit about how it works.

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6 Chapter 6
