



## PhD Study Plan

**Name:** Jane Doe

**Kennitala:** 020593–5291

**Degree Program:** Chemistry

**PhD studies start date:** 9<sup>th</sup> of January 2020

**Doctoral Committee:** (Not) Appointed by the Faculty Council  
Prof. Person1 Lastname1, Designation, University of Iceland (supervisor)  
Prof. Person2 Lastname2, Designation, University of Iceland  
Dr. Person3 Lastname3, Designation, Affiliation

**Funding status:** Lots of money from blah

**Midway evaluation:** Not completed, tentatively in the Spring of 2021

**Midway presentation:** Not completed, tentatively in the Spring of 2021

**Student background:**

The quick brown fox jumps over the lazy dog. Jackdaws love my big Sphinx of Quartz. Pack my box with five dozen liquor jugs.

The five boxing wizards jump quickly. Sympathizing would fix Quaker objectives. Many-wived Jack laughs at probes of sex quiz.

### Prior publications

#### Articles

Albert Einstein. “Zur Elektrodynamik bewegter Körper. (German) [On the electrodynamics of moving bodies]”. In: *Annalen der Physik* 322.10 (1905), pp. 891–921. DOI: <http://dx.doi.org/10.1002/andp.19053221004>.

#### Books

Paul Adrien Maurice Dirac. *The Principles of Quantum Mechanics*. International series of monographs on physics. Clarendon Press, 1981. ISBN: 9780198520115.

### Research Project(s)

#### Awesome Project I

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## References

- [1] Paul Adrien Maurice Dirac. *The Principles of Quantum Mechanics*. International series of monographs on physics. Clarendon Press, 1981. ISBN: 9780198520115.
- [2] Albert Einstein. "Zur Elektrodynamik bewegter Körper. (German) [On the electrodynamics of moving bodies]". In: *Annalen der Physik* 322.10 (1905), pp. 891–921. DOI: <http://dx.doi.org/10.1002/andp.19053221004>.
- [3] Donald Knuth. *Knuth: Computers and Typesetting*. URL: <http://www-cs-faculty.stanford.edu/~uno/abcde.html>.
- [4] Donald E. Knuth. "Fundamental Algorithms". In: Addison-Wesley, 1973. Chap. 1.2.

## Time Schedule

### First Year

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### Second Year

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### Third Year

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**Estimated Defense Date: August 2023**

### Doctoral Dissertation

The thesis will consist of a series of peer reviewed papers published in leading journals within the interdisciplinary fields relevant to the projects described. The thesis book shall also include a self-contained introduction and coherent rationale for the project and state of the art techniques to put the work in context. A tentative table-of-contents is as follows:

- Motivation
- Introduction
- Methods
- Results
- Conclusions and Future Directions
- Summary of Papers
- Full-text of papers
- References

**Prerequisite courses:** Total Credits: 0

**Course Plan:** Total Credits: 32.5  
*Autumn 2018*  
EFN115F Computational Chemistry  
*Summer 2020*  
1023 CAMD Summer School

All course descriptions are presented in an appendix.



In Reykjavik, November 26, 2020

Student  
Jane Doe

Advisor  
Person1 Lastname1

Committee members  
Person2 Lastname2  
Person3 Lastname3

**Confirmed by:**

Faculty Graduate Studies Committee Representative



## Appendix - Course Descriptions

### Courses taken at the University of Iceland

#### EFN115F - Computational Chemistry (10 ECTS)

Introduction to methodology and tools for studying the structure of molecules, chemical bonding and chemical reactions. A survey of computational approaches for calculating electron distribution such as ab initio methods (Hartree-Fock, configuration interaction, perturbation theory), density functional theory (various functional approximations) and semi-empirical methods will be given. Methods for calculating dynamics of atoms in molecular vibration and chemical reactions. The goal is to make students capable of using research level tools and carry out simple calculations related to their research interests.

- Basic concepts of quantum mechanics, variational calculations, Hartree- Fock approximation for electronic systems and basis sets
- Post Hartree-Fock methods (Moller-Plesset perturbation theory and configuration interaction)
- Density functional theory (local density approximation, gradient dependent functionals, self-interaction correction)
- Semi-empirical methods
- Normal modes of vibration, transition state theory and harmonic transition state theory, tunneling.

### External Courses

#### 1023 CAMD Summer School (5 ECTS)

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