PhD Study Plan

Name: Jane Doe

Kennitala: 020593–5291

Degree Program: Chemistry

PhD studies start date: 9th 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 backgroud:

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	Advisor	Committee members
Jane Doe	Person1 Lastname1	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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