

## Theoretical and Computational Chemistry Ph. D. Educational Plan and Timeline

The following is a typical sequence for a Ph. D. in Theoretical and Computational Chemistry (TCC), a tailor-made unique (fast-track) bachelors-to-Ph. D. program, based on 66 units including core classes, electives, and research.

**Table 1: Course sequence**

<b>First Semester (Fall)</b>		
Course	Description	Hours
CHEM 6343: Advanced Computational Chemistry	Core Course	3
CHEM 6335: Chemical Communications in Computational Chemistry	Core Course	3
CHEM 6115: Theory of the Chemical Bond	Core Course	1
CHEM 7111: Teaching Practicum	TAship	1
CHEM 6120: Current Topics in Research	Chemistry Seminar	1
	<b>Total units</b>	<b>9</b>
<b>Second Semester (Spring)</b>		
Course	Description	Hours
CHEM 6325: Introduction to ab initio Calculations - Hartree Fock Theory	Core Course	3
CHEM 6326: Density Functional Theory – Methodology and Application	Core Course	3
CHEM 7151: Research	Research	1
CHEM 7112: Teaching Practicum	TAship	1
CHEM 6121: Current Topics in Research	Chemistry Seminar	1
	<b>Total units</b>	<b>9</b>
<b>Third Semester (Fall)</b>		
Course	Description	Hours
CHEM 6341: Advanced Models and Concepts in Chemistry <sup>*)</sup>	Core Course	3
CHEM 6344: Computer Assisted Drug Design – Fundamentals and Applications <sup>*)</sup>	Core Course	3
CHEM 7351: Research	Research	2
CHEM6120: Current Topics in Research	Chemistry Seminar	1
	<b>Total units</b>	<b>9</b>
<b>Fourth Semester (Spring)</b>		
Course	Description	Hours
Elective course (see list) or CHEM 7308: Special Topics	Elective Course or Contemporary topics	3
CHEM 7351: Research	Research	3
CHEM 7251: Research	Research	2
CHEM 6121: Current Topics in Research	Chemistry Seminar	1
	<b>Total units</b>	<b>9</b>
<b>Fifth Semester (Fall)</b>		
Course	Description	Hours
Elective course (see list) or CHEM 7308: Special Topics	Elective Course or Contemporary topics	3
CHEM 7351: Research	Research	3
CHEM 7251: Research	Research	1
CHEM 6120: Current Topics in Research	Chemistry Seminar	2
	<b>Total units</b>	<b>9</b>

<b>Sixth Semester (Spring)</b>		
Course	Description	Hours
CHEM 7351: Research	Research	3
CHEM 7251: Research	Research	2
CHEM 7122: Meeting Presentation	Conference presentation	1
CHEM 7233: Research Synopsis	Qualifying examination (both written and oral)	2
CHEM 6121: Current Topics in Research	Chemistry Seminar	1
	<b>Total units</b>	<b>9</b>
<b>Seventh Semester (Fall) Ph.D. candidacy</b>		
Course	Description	Hours
CHEM 8698: Dissertation	PhD thesis work	6
	<b>Total units</b>	<b>6</b>
<b>Eighth Semester (Spring)</b>		
Course	Description	Hours
CHEM 8698: Dissertations	Dissertation	6
	<b>Total units</b>	<b>6</b>

<sup>\*)</sup> Due to the diverse range of graduate students participating in the TCC Ph. D. program, individual students may exchange these core courses with additional electives that more precisely cover their research focus with approval from their PI.

**Selection of current electives (the list is frequently extended/modified according to the individual needs of the diverse graduate student population)**

### Courses from the chemistry department

- CHEM 6345 Going Beyond Hartree-Fock: Electron Correlation Methods
- CHEM 6346 Calculation of Molecular Properties
- CHEM 6348 Statistical Molecular Thermodynamics
- CHEM 5308 Special Topics; crystallography

### Courses from other department/schools

- MATH 6350 Mathematical Models in Biology
- MATH 6370 Parallel Scientific Computing
- CS 7320 Artificial Intelligence
- CS 7324 Machine Learning in Python
- CS 7311 Foundations of Computing
- CS 7345 - Advanced Application Programming
- CS 8320 Knowledge-Intensive Problem-Solving
- CS 8321 - Machine Learning and Neural Networks
- DS 7331 Machine Learning I
- DS 7335 Machine Learning II
- ITOM 6217 Data Mining and Machine Learning

**Table 2: Summary of Classes**

Courses	Hours
Core Courses	19
Electives/Special Topics	6
Research	18
Conference Presentation	1
Research Synopsis	2
Dissertation	12
Teaching Practicum	2
Current Topics in Research	6
<b>TOTAL</b>	<b>66</b>

A successful dissertation usually includes at least 4-5 research papers that have been published in peer-reviewed scientific journals.