

Computational Chemistry and Chemical Physics

The Computational Chemistry & Chemical Physics concentration is an interdisciplinary field at the crossroads of chemistry and physics and is administered jointly by the Chemistry and Physics Departments. The concentration provides students with a broad-based understanding in fundamental molecular sciences, as well as a background for graduate studies in physical chemistry, chemical physics, or molecular engineering. Concentrators are required to take twenty courses in chemistry, physics, computational science, and mathematics, although approved courses in applied mathematics, biology, geological sciences, or engineering may be substitutes. Computational Chemistry & Chemical Physics concentrators are also advised to take at least six courses in the humanities and social sciences. Computational Chemistry & Chemical Physics concentrators at all levels (first-year through seniors) are actively involved in research with faculty members in both departments.

Standard program for the Sc.B. degree

Twenty semester courses in chemistry, physics, and mathematics, with a minimum of three semester courses in mathematics. Core courses are:

Foundational Coursework ¹

CHEM 0330	Equilibrium, Rate, and Structure	1
CHEM 0350	Organic Chemistry I	1
CHEM 0500	Inorganic Chemistry	1
PHYS 0070	Analytical Mechanics	1
PHYS 0470	Electricity and Magnetism	1

One Foundational Computation Course

CSCI 0111	Computing Foundations: Data	1
CSCI 0150	Introduction to Object-Oriented Programming and Computer Science	1
CSCI 0170	Computer Science: An Integrated Introduction	1
CSCI 0190	Accelerated Introduction to Computer Science	1
DATA 0250	Applied Statistics in Python	1
DATA 1030	Hands-on Data Science	1
DATA 1050	Data Engineering	1
APMA 0160	Introduction to Scientific Computing	1
APMA 0200	Introduction to Modeling	1

One Experimental or Computational Laboratory Course

CHEM 1560K	Computational Chemistry ²	1
CHEM 1560Q	Accelerating Chemical Discovery ²	1
PHYS 1600	Computational Physics ²	1
PHYS 1640	Introduction to Computational Physics and Data Analysis ²	1
CHEM 1160	Physical Chemistry Laboratory ³	1
PHYS 0560	Experiments in Modern Physics ³	1
PHYS 1560	Modern Physics Laboratory ³	1

One Quantum Mechanics Course

PHYS 1410	Quantum Mechanics A (Select One: Quantum Mechanics)	1
CHEM 1140	Physical Chemistry: Quantum Chemistry (Select one: Quantum Mechanics)	1

One Statistical Mechanics Course

CHEM 1150	Physical Chemistry: Thermodynamics and Statistical Mechanics	1
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PHYS 1530	Thermodynamics and Statistical Mechanics	3
Three Mathematics Courses ⁴		3
MATH 0190	Single Variable Calculus, Part II (Physics/Engineering)	3
MATH 0200	Multivariable Calculus (Physics/Engineering)	3
MATH 0520	Linear Algebra	3
Six courses, primarily at the 1000 or 2000 level, in chemistry, physics or computer science.		6
Two Semesters of Independent Study		2
PHYS 1990	Senior Conference Course	2
CHEM 0980	Undergraduate Research	2
Total Credits		20

¹ Students can continue to replace these courses with more advanced chemistry and physics courses if they have satisfied the prerequisites.

² Recommended for students interested in molecular modeling.

³ Recommended for students interested in experimental chemical physics.

⁴ Students can replace these courses with more advanced mathematics courses if they have satisfied the prerequisites.

Requirements for Honors

All Computational Chemistry and Chemical Physics concentrators who have grades of A or S with distinction in a majority of their concentration courses will be considered for Honors; no separate application is necessary.

The requirements for Honors in Computational Chemistry and Chemical Physics are:

* Grades of A or S with distinction in a majority of courses taken for the concentration.

* Two semesters of Independent Study (CHEM 0980 or equivalent). Guidelines and requirements associated with Independent Study are in the Undergraduate Concentration Handbook which can be found at the department website (<http://www.brown.edu/academics/chemistry/undergraduate/>).

* A Thesis in a form approved and recommended by the research advisor. Additional information about thesis guidelines will be provided to seniors by the Concentration Advisor.

* A Poster presentation at the chemistry department's spring undergraduate poster session and presentation at the end-of-year thesis presentations.