

Course Change Request

New Course Proposal

Date Submitted: 04/10/26 2:21 pm

Viewing: **CSI 686 : Molecular Dynamics Modeling**

Last edit: 04/13/26 9:44 am

Changes proposed by: blaisten

Are you completing this form on someone else's behalf?

No

Effective Term: Fall 2026

Subject Code: CSI - Computational Science & Informatics

Course Number: 686

Bundled Courses:

Is this course replacing another course? Yes

Old Course Number: CSI 786 - Molecular Dynamics Modeling

Equivalent Courses:

Catalog Title: Molecular Dynamics Modeling

Banner Title: Molecular Dynamics Modeling

Will section titles vary by semester? No

Credits: 3

Schedule Type: Lecture

Hours of Lecture or Seminar per week: 2.67

In Workflow

1. CDS Chair
2. SC Curriculum Committee
3. SC Assistant Dean
4. Assoc Provost-Graduate
5. Registrar-Courses
6. Banner

Approval Path

1. 04/10/26 5:46 pm
Arie Croitoru
(acroitor): Approved for CDS Chair

Repeatable: May only be taken once for credit, limited to 2 attempts (N2) **Max Allowable Credits:**
3

Default Grade Mode: Graduate Regular

Recommended Prerequisite(s):
CSI 690 or CHEM 633 or permission of instructor.

Recommended Corequisite(s):

Required Prerequisite(s) / Corequisite(s) (Updates only):

Registrar's Office Use Only - Required Prerequisite(s)/Corequisite(s):

And/Or	(Course/Test Code	Min Grade/Score	Academic Level)	Concurrency?

Registration Restrictions (Updates only):

Registrar's Office Use Only - Registration Restrictions:

Field(s) of Study:

Class(es):

Level(s):

Degree(s):

School(s):

Catalog Description:

Introduces simulation methods in physical chemistry sciences. Covers computational approaches to modeling molecular and condensed matter systems, including interatomic and molecular potentials, Molecular Dynamics methods, time averages, ensemble distributions, numerical sampling, thermodynamic functions, response theory, transport coefficients, and dynamic structure. Classical and quantum approaches are discussed.

Justification:

What: Creating a new course to replace an existing course.

Why: This is a renumbering of the existing course CSI 786.

Does this course cover material which crosses into another department? No

Learning Outcomes:

Will this course be scheduled as a cross-level cross listed section? No

Attach Syllabus

[CSI686_syllabus.pdf](#)

Additional Attachments

Staffing:

Dr. Estela Blaisten, who is the creator of CSI 786 (to be discontinued) is a professor in the College of Science, Department of Computational and Data Sciences.

Relationship to Existing Programs:

Computational Sciences and Informatics, PhD

Computational Science, MS

Quantum Science and Engineering, MS

Relationship to Existing Courses:

CSI 786 Molecular Dynamics Modeling - This course will be discontinued.

BINF 741 Introduction to Computer Simulations of Biomolecules. This course focuses on molecular dynamics and Monte Carlo algorithms specifically applied to biomolecules, including protein docking and simulations.

Have you reached out to the Libraries to determine whether there are adequate resources to support your course? If not, please email Meg Meiman, Associate University Librarian for Learning, Research, and Engagement at mmeiman2@gmu.edu.

Yes

Additional Comments:

Reviewer Comments

CSI 686 *Molecular Dynamics Modeling*

Instructor Name: Estela Blaisten

Email address: blaisten@gmu.edu

Department: Computational and Data Sciences

The theme of the course is the Molecular Dynamics methodology. These methods are currently orthodox means for simulating molecular-scale models of matter including nano systems, bulk crystals, glasses, liquids, polymers, surfaces and interfaces, and biomaterials. The methodology has been adopted by computational chemists, physicists, engineers, biologists, geophysicists and is today an essential element of bio-oriented research.

By the end of this course, students will be able to

1. Use Molecular Dynamics algorithms for implementing numerical simulations in computational science that solve a given problem at the atomic level.
2. Appraise theoretical foundations, applicability, and use of algorithms employed in the simulations.
3. Reinforce practical skills for designing and building computer programs or scripts that include dedicated data analysis of the simulation results learned in class.
4. Perform elementary atomistic simulations.

Prerequisites: Calculus, introductory physics or physical chemistry, and knowledge of a programming language (at the level of CSI 501, or better). Understanding of the basic concepts of ordinary differential equations is helpful.

Required Textbook

The Art of Molecular Dynamics Simulation (2nd ed), Dennis Rapaport, Cambridge U. Press, 2011.

Supplemental textbook:

Ab Initio Molecular Dynamics: Basic Theory and Advanced Methods, Cambridge U. Press, 2010.

Course schedule

Week 1: Numerical methods in science, stochastic vs. deterministic. Modeling vs. simulation. “Experiments” in the computer.

Week 2: Newtonian or Hamiltonian dynamics. Phase space. Distribution functions. Sampling theory. Periodic boundary conditions.

Week 3: Classical models of different bonds. Model potentials. How to assess predictability. Finite difference methods for the solution of ordinary differential equations.

Week 4: Algorithms for Molecular Dynamics. Reliability of trajectories.

Week 5: How to perform Molecular Dynamics simulations. Equilibration. Production, Data analysis of trajectories.

Week 6: Static properties. Thermodynamic functions. Thermodynamic response functions. Entropic functions. Static structure.

Week 7: Dynamic properties. Time correlation functions. Transport coefficients. Dynamic structure.

Week 8: Ehrenfest molecular dynamics. Born–Oppenheimer molecular dynamics. Car–Parrinello molecular dynamics

Week 9: Hellmann–Feynman forces. Electronic structure methods. Exchange and correlation energy. Plane waves

Week 10: Pseudopotentials. Hybrid QM/MM molecular dynamics.

Week 11: Applications to solids, minerals, polymers, aqueous solutions.

Week 12: Projects pre-presentation by individual students.

Week 13 (last class): Projects pre-presentation in sequential fashion

Week 14 (final exam day): Each student does a final presentation of his/her project (this is not an exam)

Grading scale: A+, A, A- (90-100), B+, B, B- (80-89), C (70-79), F (< 70).

Slight variations are possible depending upon the overall student performance in the class.

- 1) Homework (40%). A set of 8-10 homework presented in a report-like fashion.
- 2) Individual project (30%).
- 3) Class participation and attendance (30%). Includes presentations by students on the material related to the textbooks or class notes, on their advances in the individual project, or additional explanations on homework assignments. Participation also includes a final presentation of the individual project.
- 4) There are no exams: neither mid-term nor final.

Other considerations:

- 1) If there are personal obligations related to religious holidays, please inform the instructor the first week of class.
- 2) Disability-related accommodations require pertinent written communication with the instructor the first week of class. [<http://ds.gmu.edu/>]

Course Policies:

1. **Email:** Students are responsible for reading and maintaining the content of university emails sent to their GMU email account.
2. **Academic integrity:** Students must adhere to the GMU Academic Standards Code, be very respectful of the class co-participants and the instructor. Students are responsible for their own work and must take on the responsibility of dealing explicitly with consequences

to any academic integrity violation. [<https://academicstandards.gmu.edu/academic-standards-code/>]

3. **University policies:** Students must follow the university policies including the responsible use of computing [, <http://universitypolicy.gmu.edu>], <http://universitypolicy.gmu.edu/policies/responsible-use-of-computing>].
4. **AI use** is allowed in the course but not encouraged. Students must report the use of AI in their homework/projects.
5. **Family Educational Rights and Privacy Act (FERPA):** The Family Educational Rights and Privacy Act of 1974 gives protection to student educational records and provides students with certain rights. [<http://registrar.gmu.edu/privacy>].