George Mason University  
Graduate Course Approval/Inventory Form  

Please complete this form and attach a copy of the syllabus for new courses. Forward it as an email attachment to the Secretary of the Graduate Council. A printed copy of the form with signatures should be brought to the Graduate Council Meeting. Complete the Coordinator Form on page 2, if changes in this course will affect other units.

Please indicate: □ X NEW □ MODIFY □ DELETE

Local Unit: SCS

Graduate Council Approval Date:

Course Designation: NANO

Course Number: 620

Full Course Title: Computational Modeling in Nanoscience

Abbreviated Course Title (24 characters max.): Computational Nanoscience

Credit hours: 3

Program of Record: Graduate Certificate in Nanotechnology and Nanoscience

Repeatable for Credit? D=Yes, not within same term Up to ___ hours maximum

T=Yes, within the same term Up to ___ hours maximum

N=Cannot be repeated for credit

Activity Code (please indicate): □ X Lecture (LEC) □ Lab (LAB) □ Recitation (RCT)

□ Studio (STU) □ Internship (INT) □ Independent Study (IND) □ Seminar (SEM)

Catalog Credit Format 3: 3: 0

Course Level: GF(500-600) □ X GA(700+)

Maximum Enrollment: 30

For NEW courses, first term to be offered: S05

Prerequisites: NANO 500, 510, and 520, and admission into the Graduate Certificate in Nanotechnology and Nanoscience.

Catalog Description (35 words or less): Introduction to simulation methods used in nanoscience. Covers computational approaches to modeling molecular and condensed matter at the nanoscale level, including interatomic and molecular potentials; molecular mechanics; molecular dynamics; monte carlo averaging; ensemble distributions; numerical sampling; thermodynamic functions; dynamic structure; and an introduction to cellular automata.

APPROVAL SIGNATURES:

Submitted by: ________________________________ email: ________________

Department/Program: ________________________________ Date: __________________

College Committee: ________________________________ Date: __________________

Graduate Council Representative: ________________________________ Date: __________________
**GEORGE MASON UNIVERSITY**  
**Course Coordination Form**

**Approval from other units:**

Please list those units outside of your own who may be affected by this new, modified, or deleted course. Each of these units must approve this change prior to its being submitted to the Graduate Council for approval.

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Graduate Council approval: ________________________________ Date: ____________

Graduate Council representative: __________________________ Date: ____________

Provost Office representative: _____________________________ Date: ____________
1. COURSE DESIGNATION:

NANO 620 Computational Modeling in Nanoscience (3: 0: 0)

Prerequisites: NANO 500, 510, and 520, and admission into the Graduate Certificate in Nanotechnology and Nanoscience.

Catalog description: Introduction to simulation methods used in nanoscience. Covers computational approaches to modeling molecular and condensed matter at the nanoscale level, including interatomic and molecular potentials; molecular mechanics; molecular dynamics; monte carlo averaging; ensemble distributions; numerical sampling; thermodynamic functions; dynamic structure; and an introduction to cellular automata.

Course Grading: Standard grading options for a graduate course.

2. COURSE JUSTIFICATION:

Course objectives: Students will learn the computational methods used in nanoscience simulations.

Course necessity: This course is needed in order to provide students with exposure to the specialized computational techniques and methods that are especially relevant for the simulation of the physical processes operative in nanoscience systems.

Relationship to existing programs: The proposed course serves as part of the sequence of classes applicable to the Graduate Certificate in Nanotechnology and Nanoscience. It offers specialized training in computational modeling that is not offered in other courses.

Relationship to existing courses: No other similar course is currently offered at GMU.

3. APPROVAL HISTORY NA

4. SCHEDULING AND PROPOSED INSTRUCTORS

Time of initial offering: Spring 05

Proposed instructors: Dr. Estela Blaisten-Barojas or another member of the Nanotechnology faculty.
5. SAMPLE STUDENT SYLLABUS:

NANO 620 Computational Modeling in Nanoscience

Textbooks:

Akhiesh Lakhatakia “Handbook of nanometer structures their modeling and simulation,” SPIE Press

Tentative Course Content:

- Week 1: Introduction to nanoscience simulations
- Week 2: Simulation requirements in the nanoregime
- Week 3: Schrodinger wave function coupled to Poisson equation techniques
- Week 4: Atoms and interatomic potentials.
- Week 5: Molecular Modelers.
- Week 6: Monte Carlo techniques
- Week 7: Numerical sampling and combinatorial sampling
- Week 8: Ensemble distributions
- Week 9: Molecular Optimizers for condensed systems
- Week 10: Thermodynamics in the nanoscale
- Week 11: Quantum structures and surfaces. Finite Size effects
- Week 12: Cellular automata
- Week 13: Quantum mechanical approaches for time-dependent nonlinear device physics
- Week 14: Introduction to modified ensemble Monte Carlo techniques.

Grading: Assignments: 30%; Midterm 30%; Final: 40%