George Mason University–Office of the Registrar **Undergraduate Course Approval Form**

Please complete this form and attach a copy of the syllabus and catalog description for new courses. Forward the form and attachments to your departmental curriculum committee for approval, and then to your College/School curriculum committee, or Dean's office, for final approval. The approved form should then be forwarded to the Academic Scheduling Office, MS 3D1. This is for ***undergraduate course approval only***. Please see the Provost Office/Graduate Council website to obtain a copy of the Graduate Course Approval Form and for details about the graduate course approval process.

Note: Colleges and Schools are responsible for submitting new or modified catalog descriptions (35 words or less, using catalog format) to Creative Services by deadlines outlined in the yearly Catalog production calendar.

Please indicate: **New** X **Modify** _____ **Delete** _____

Department/Unit: CDS **Course Subject/Number:** CDS 487

Submitted by: D.A. Papaconstantopoulos **Ext:** 3-3624 **Email:** dpapacon@gmu.edu

Course Title: Electronic Structure Computations

Effective Term (New/Modified Courses only)**:** Spring 2009 **Final Term** (deleted courses only)**:** _____

Credit Hours: (Fixed) 3 (Var.) _____ to _____ **Grade Type** (check one)**:**

X Regular graduate (A, B, C, etc.)
_____ Satisfactory/No Credit only
_____ Special graduate (A, B, C, etc. + IP)

Repeat Status* (check one): ____ **NR**-Not repeatable ____ **RD**-Repeatable within degree ____ **RT**-Repeatable within term

***Note: Used only for special topics, independent study, or internships courses** **Total Number of Hours Allowed:** _____

Schedule Type Code(s): 1. LEC **LEC**=Lecture **SEM**=Seminar **STU**=Studio **INT**=Internship **IND**=Independent Study
2. _____ **LAB**=Lab **RCT**=Recitation (second code used only for courses with Lab or Rct component)

Prereq X **Coreq** ___ (Check one)**:** PHYS 308 or PHYS 402

Note: Modified courses - review prereq or coreq for necessary changes; Deleted courses - review other courses to correct prereqs that list the deleted course.

Description of Modification (for modified courses)**:** _____

Special Instructions (major/college/class code restrictions, if needed)**:** _____

***Approval Signatures*:**

Department or Unit: _____ **Date:** _____
(Signature)

College/School Committee: _____ **Date:** _____
(Signature)

Approval from other units for CDS 487:

Please list those units outside of your own which may be affected by this new, modified, or deleted course. Each of these units should approve this action prior to its being submitted to the COS Curriculum Committee for approval.

Unit:	Head of Unit's Signature:	Date:
Unit:	Head of Unit's Signature:	Date:
Unit:	Head of Unit's Signature:	Date:
Unit:	Head of Unit's Signature:	Date:
Unit:	Head of Units Signature:	Date:

COS Curriculum Committee approval: _____ Date: _____

Course Proposal Submitted to the COS Curriculum Committee

1. COURSE NUMBER AND TITLE:
CDS 487 Computational Materials Science

Course Prerequisites:
PHYS 308 or PHYS 402, proficiency in computer programming

Catalog Description:
The course covers computational aspects of materials science, such as first-principles methods of electronic structure calculations of periodic solids, clusters, and molecules as well as the use of empirical potentials. Examples will be drawn from metals, insulators, and semiconductors. The students will be directed to construct simple codes and be guided in the use of the more sophisticated available computational packages.

2. COURSE JUSTIFICATION:

Course Objectives:

This course will cover first introductory information on crystallography to prepare the students with the necessary background for computing the electronic structure of solids. In addition a review of quantum mechanics will be presented intended to lead to a demonstration that the Schrodinger equation can be solved analytically only for the hydrogen atom. For the rest of the elements in the periodic table numerical solutions are possible. Such approaches will be discussed using plane wave or tight-binding techniques. The students will be expected to write programs of simplified versions of such methods, and will be introduced in the use of more sophisticated packages provided by the instructor.

Course Necessity:

This is one of the advanced courses of the B.S. degree in Computational and Data Sciences that combines methodology and application in the physics track of the program.

Course Relationship to Existing Programs: No relationship

Course Relationship to Existing Courses:

This course is a lower level treatment of material taught in the graduate course CSI 787.

3. APPROVAL HISTORY:

4. SCHEDULING AND PROPOSED INSTRUCTORS:

Semester of Initial Offering: Spring 2009

Proposed Instructors: Dr. Papaconstantopoulos

5. TENTATIVE SYLLABUS: See attached.

COURSE NUMBER
COURSE TITLE

-- SYLLABUS --

Prerequisites:

PHYS 308 or PHYS 402, proficiency in computer programming

Credits: (3)

Instructor: D. Papaconstantopoulos

Office Hours: TBD

Course Description:
The course covers computational aspects of materials science, such as first-principles methods of electronic structure calculations of periodic solids, clusters, and molecules as well as the use of empirical potentials. Examples will be drawn from metals, insulators, and semiconductors. The students will be directed to construct simple codes and be guided in the use of the more sophisticated available computational packages.

Lecture Content:

Lecture 1: Introductory concepts on crystal structures:
Periodicity in crystals, symmetry operations, units' cells,
two and three dimensional lattices.

Lecture 2: Definitions of primitive lattice vectors and description
of the cubic and hexagonal crystal structures.

Lecture 3: The concept of the reciprocal lattice and Brillouin zones.

Lecture 4: The Schrodinger equation:
Solution for the Hydrogen atom and connection to the Bohr model.

Lecture 5: The concept of the energy band and the density of states.

Lecture 6: The tight-binding approach and the free-electron model.

Lecture 7: Applications of tight-binding methodology to a chain of atoms,
and a square lattice. Simple applications to three dimensions.

Lecture 8: The second moment approximation, its applications and limitations.

Lecture 9: Classical approaches to calculating the cohesive energy using
interatomic potentials.

Lecture 10-15: The students will be directed to construct simple computer codes
and will be guided in the use of one of the available computational
packages in materials science.

Homework: In the first part of the course there will be mainly problems solved using analytical approaches. In the second part the homework assignments will be related to the project.

Project: The project will have two components. Writing code for simple applications of materials theories, and using commercial packages to obtain and analyze the results.

Exams: There will be a midterm exam but no final exam.

Grades:

Homework (20%), Projects (60%), Midterm (20%)

Required Texts:

References

D.A. Papaconstantopoulos, Handbook of the Band Structure of Elemental Solids, Plenum Press 1986.

D.A. Papaconstantopoulos, and M.J. Mehl, Tight-binding Method in Electronic Structure, "Encyclopedia of Solid State Physics", p194,Vol.6, Elsevier (2005).