COURSE SPECIFICATIONS

Form

Course Title: **Modelling and molecular dynamics simulations at the nanoscale**

Course Code: **23066102-2**

Date: 2018 – 12 – 28	**Institution**: Umm Al-Qura University
College: Al-Jamoum University College	**Department**: Physics

A. Course Identification and General Information

1. Course title and code: **Modelling and molecular dynamics simulations at the nanoscale (23066102-2)**
2. Credit hours: **2 credit hours.**
3. Program(s) in which the course is offered: **Nano physics Program, Al-Jamoum University College.** (If general elective available in many programs indicate this rather than list programs)
4. Name of faculty member responsible for the course:
5. Level/year at which this course is offered: **2nd Level.**
6. Pre-requisites for this course (if any): **-**
7. Co-requisites for this course (if any): **-**
8. Location if not on main campus: **Al-Jamoum University College.**
9. Mode of Instruction (mark all that apply):

a. Traditional classroom	✓	percentage?	70%
b. Blended (traditional and online)		percentage?	
c. E-learning	✓	percentage?	30%
d. Correspondence		percentage?	
e. Other:		percentage?	

Comments:

B. Objectives

1. The main objective of this course

The student should be trained on the basic knowledge about the computer methods of simulation and modelling used at present to study systems of nanometric size.
Moreover, the student should become familiar with the use of standard software packages in which this type of methods are relevant and should master their possible applications and limitations.

2. Describe briefly any plans for developing and improving the course that are being implemented. (e.g. increased use of the IT or online reference material, changes in content as a result of new research in the field)

In this context, the module focus on the connection of current research activities in nanoscience to their potential technological application.

C. Course Description (Note: General description in the form used in the program's bulletin or handbook)

Course Description:

The subject will be divided in two great blocks, one due to the simulations of molecular dynamics and a second one aimed to the description of the methods of first principles used in the Nano-structure modelling.

1. Topics to be Covered

List of Topics	No. of Weeks	Contact hours
Introduction to ab-initio methods in the modelling of nanostructures.	2	2
Solid-state methods..	3	6
Quantum physics methods.	3	6
Introduction to molecular dynamics simulation in the nanoscale.	2	4
The concept of forcefield.	2	4
Needed algorithms.	2	4
Mesoscopic methods.	2	4

2. Course components (total contact and credit hours per semester):

		Lecture	Tutorial	Laboratory/ Studio	Practical	Other	Total
Contact Hours	Planned	30					30
	Actual	30					30
Credit	Planned	1					2
	Actual	1					2

3. Individual study/learning hours expected for students per week.

4. Course Learning Outcomes in NQF Domains of Learning and Alignment with Assessment Methods and Teaching Strategies

On the table below are the five NQF Learning Domains, numbered in the left column.

First, insert the suitable and measurable course learning outcomes required in the appropriate learning domains (see suggestions below the table). **Second**, insert supporting teaching strategies that fit and align with the assessment methods and targeted learning outcomes. **Third**, insert appropriate assessment methods that accurately measure and evaluate the learning outcome. Each course learning outcomes, assessment method, and teaching strategy should fit in together with the rest to form an integrated learning and teaching process. (Courses are not required to include learning outcomes from each domain.)

Curriculum Map

Code #	NQF Learning Domains And Course Learning Outcomes	Course Teaching Strategies	Course Assessment Methods
1.0	**Knowledge**		
1.3	The process and mechanisms supporting the structure and function are specific topics.		
1.4	Related terminology, numbering and classification systems.		
1.6	Knowledge development related to the program.		
2.0	**Cognitive Skills**		
2.2	Analyzing, evaluating and interpreting relevant qualitative and quantitative scientific data.		

2.3	Develop the argument and divorce the appropriate judgments according to scientific theories and concepts.		
3.0	**Interpersonal Skills & Responsibility**		
3.2	Application of techniques and tools related to scientific ethics.		
4.0	**Communication, Information Technology, Numerical**		
4.1	Use information and communication technology effectively		
4.3	Think independently, assign tasks and solve problems on a scientific basis.		
4.5	Taking into account societal problems associated with customs, traditions and ethics.		
4.6	Ability to learn self and continuously.		
4.7	Apply models, scientific systems and tools effectively.		

5. Assessment Task Schedule for Students During the Semester

	Assessment task (i.e., essay, test, quizzes, group project, examination, speech, oral presentation, etc.)	Week Due	Proportion of Total Assessment
1	1st Quiz.	7	10
2	2nd Quiz.	11	10
3	1st Homework (E-Learning).	4	10
4	2nd Homework (E-Learning).	8	10
5	Research.	12	20
6	Final written Examination.	16	40

D. Student Academic Counseling and Support

1. Arrangements for availability of faculty and teaching staff for individual student consultations and academic counseling. (include the time teaching staff are expected to be available per week)

Academic advising hours for guidance are included in the faculty member schedule of 4 hours per week.

E. Learning Resources

1. List Required Textbooks

Computer Simulation of Liquids, M.P. Allen D.J. Tildesley, Oxford Science Publications, 2nd edition (2017).

Modelling Molecular Structures, A. Hinchliffe, Wiley and Sons, (2000).

Computational Materials Science, K. Ohno, K. Esfarjani, and Y. Kawazoe Springer, Berlin, 2nd edition (2018).

Electronic structure: basic theory and practical methods, Richard M. Martin, Cambridge University Press, (2004)

2. List Essential References Materials (Journals, Reports, etc.)

3. List Electronic Materials, Web Sites, Facebook, Twitter, etc.

4. Other learning material such as computer-based programs/CD, professional standards or regulations and software.

F. Facilities Required

Indicate requirements for the course including size of classrooms and laboratories (i.e. number of seats in classrooms and laboratories, extent of computer access, etc.)

1. Accommodation (Classrooms, laboratories, demonstration rooms/labs, etc.)

Class room for 10 students.
2. Technology resources (AV, data show, Smart Board, software, etc.) The class room should be equipped with a pc and data-show.
3. Other resources (specify, e.g. if specific laboratory equipment is required, list requirements or attach list)

G. Course Evaluation and Improvement Procedures

1. Strategies for Obtaining Student's Feedback on Effectiveness of Teaching **Questioners.**
2. Other Strategies for Evaluation of Teaching by the Instructor or the Department **Using course report.**
3. Procedures for Teaching Development **Using course report.**
4. Procedures for Verifying Standards of Student's Achievement (e.g. check marking by an independent member teaching staff of a sample of student's work, periodic exchange and remarking of tests or a sample of assignments with staff members at another institution) **A random sample of students' assessments is corrected through the committee formed by the department.**
5. Describe the planning arrangements for periodically reviewing course effectiveness and planning for developing it. **Review stakeholders and conduct periodic questioners.**

Name of Course Instructor: _____

Signature: _____ Date Completed: _____

Program Coordinator: _____

Signature: _____ Date Received: _____