<table>
<tr><td>New Course Code and Title</td><td colspan="3">MS7240 Modelling of Materials
(1AU)</td></tr>
<tr><td>Course Coordinator</td><td colspan="3">AP Zhao Yang</td></tr>
<tr><td rowspan="3">Details of Course</td><td colspan="3">Rationale for introducing this course

This course provides an introduction to modelling of materials, to enable students to investigate materials properties at different length and time scales in situations when experiments are not feasible or expensive.</td></tr>
<tr><td colspan="3">Aims and Objectives:
The aim of this course is to introduce some of the more important computational modelling techniques such as continuum methods, atomistic and molecular simulation, and quantum mechanics.

Students will gain insights into some fundamental, theoretical and numerical concepts through some examples which illustrate the principles.

At the end of this course the students will:

• Explain the different techniques of computational modelling of materials;
• Differentiate between the usage of Finite Element Method, Molecular Dynamics simulations, and ab-Initio quantum mechanical modelling;
• Appreciate the utility of computational modelling as an aid to uncover underlying physics of experimental studies.</td></tr>
<tr><td colspan="3">Course Syllabus
Refer to page 3 and 4</td></tr>
<tr><td rowspan="3">Assessment
(Individual Assessment)</td><td>Assessment Points</td><td colspan="2">3</td></tr>
<tr><td rowspan="2">Mode of Assessments and weighting</td><td rowspan="2">Tutorial 1: Short structured questions, Case Studies
Tutorial 2: Case studies
CA 1: Case Studies</td><td>30%

20%
50%</td></tr>
<tr><td>100%</td></tr>
</table>

	Mapping of assessment to course objectives • **LO1**: Explain the different techniques of computational modelling of materials; • **LO2**: Differentiate between the usage of Finite Element Method, Molecular Dynamics simulations, and ab-Initio quantum mechanical modelling. • **LO3**: Appreciate the utility of computational modelling as an aid to uncover underlying physics of experimental studies.	Tutorial 1: L01 and L02 Tutorial 2: L01 and L02 CA 1: All
To be offered with effect from (state Academic Year and Semester)	*AY2018/19 Semester 1*	
Cross Listing (if applicable)	*N/A*	
Prerequisites (if applicable)	*N/A*	
Preclusions (if applicable)	*N/A*	
Mode of Teaching & Learning (Lectures, regular tests, Q&A, problem-based learning)	*Lectures, Regular Tests, Simulations*	
Basic Reading List • **Compulsory Reading** • **Supplementary Reading**	Supplementary Reading: *The papers and books as mentioned in the recorded lectures and citation list.*	
Hours of Contact/Academic Units	*13 hours/ 1 AU*	

Course Syllabus
The following topics will be covered:

Module 1: Basics of Modelling and Simulation

1. Why Model and Simulate?
- Why Model & Simulate
- Examples
- Advantages of Simulations
- Drawbacks of Simulations.

2. Multiscale Modelling
- Length
- Time
- Temperature
- Energy

3. Methods of Modelling
- Process of simulation
- Types of simulation
- Software
- Coding
- Introduction to coding in Python

MODULE 2: Materials Simulation: Classical Methods

1. Finite Element Method
- Application
- Limitation
- Process

2. Molecular Dynamics
- Procedure
- Softwares
- Applications

3. Modelling Diffusion
- Heat diffusion: 1D and 2D
- Particle Diffusion
- Exciton Diffusion

MODULE 3: Materials Simulation: Quantum Methods

1. Introduction to Quantum Mechanics
- Notation in QM
- Eigenstate and Eigenvalue
- Schrödinger Equation
- Particle in a box
- Harmonic Oscillator
- Plane Waves

2. Tight Binding Model
- Direct and Reciprocal Lattice
- Principles

- Finite System Application
- Infinite Periodic System Application

3. Density Functional Theory (DFT)
- Principles
- Applications