Molecular Modelling 2019-20

1. Basic Module Data

Module Title:	Molecular Modelling
School:	School of Mathematics and Physics
Subject:	Physics
Module Code:	PHY9002M
Credit Rating:	15
Level:	Level 4
Pre-requisites:	Statistical Mechanics 2017-18
Co-requisites:	None
Barred Combinations:	None
Module Co-ordinator(s):	Matthew Watkins (MWatkins)

2. Module Synopsis

The module introduces modern computational techniques for molecular modelling in condensed matter physics.

3. Outline Syllabus

• Introduction to molecular modelling concepts, Molecular Dynamics (MD) equations, MD programs and algorithms.
• Basic Molecular Dynamics program and initialization.
• Forces calculation: Lennard-Jones potential, Stillinger-Weber potential, truncation and shift of the potential.
• Equations of motion: Taylor expansion algorithm, Verlet algorithm, Leap-frog algorithm, Beeman algorithm.
• MD analysis: radial distribution, mean square displacement
• Thermostats: Berendsen thermostat, Andersen thermostat, Nosé-Hoover Thermostat.
• Free Energy Calculation: thermodynamic integration, chemical potentials, umbrella sampling.
• Elements of Monte Carlo (MC) simulation: MC method, Metropolis method
• Simulation time economy: boundary conditions, Verlet list, cell list.
• Applications in macromolecular modelling, the force fields, molecular visualization.

4. Module Learning Outcomes

LO1	Explain main concepts of MD and MC and their applications to condensed matter physics
LO2	Design, implement and execute basic computer program relevant to the material of the syllabus.
LO3	Critical analyse problems in molecular modelling and solve them using moderns MD simulation.

5. Learning and Teaching Strategy/Methods

The total student effort for this module is 150 hours on average. This total includes: - Lectures, which introduce and discuss core concept and issues. During the lectures the students will also be directed towards recommended reading material and on-line resources. Research-informed material will be introduced as examples where appropriate. -Practical workshops, which offer the opportunity to practically apply topics covered within the lecture programme and in the module's recommended textbooks. Workshops support students to review their understanding of the module lectures, assigned readings, and applying them in the practical work involved in the assignment.

6. Assessment

The module is assessed via a composite portfolio including assessment of computational exercises, mini-project and an oral presentation.

Assessment Method	Weighting (%)	Learning Outcome(s) Tested	Group Work
Portfolio	100	LO1, LO2, LO3	No

7. Professional, Statutory and Regulatory Body Requirements

None

8. Indicative Reading

Type	Whole book
Title	Molecular modelling: principles and applications
Authors	Leach, Andrew R.
Importance	Further Reading
Date	2001
Edition	

Publisher	Pearson Education
ISBN	0582382106, 9780582382107
Type	Whole book
Title	Computer simulation of liquids
Authors	Allen, M. P., Tildesley, D. J.
Importance	Recommended Reading
Date	c1987
Edition	
Publisher	Clarendon Press
ISBN	0198556454, 9780198556459
Type	Whole book
Title	Numerical recipes: the art of scientific computing
Authors	Press, William H.
Importance	Further Reading
Date	2007
Edition	
Publisher	Cambridge University Press
ISBN	0521880688, 9780521880688
Type	Whole book
Title	Theory of simple liquids: with applications to soft matter
Authors	Hansen, Jean-Pierre, McDonald, Ian R.
Importance	Further Reading
Date	c2013
Edition	
Publisher	Academic Press
ISBN	9780123870339, 9780123870322
Type	Whole book
Title	Atomistic computer simulations: a practical guide
Authors	BraÌ•zdovaÌ•, Veronika, Bowler, D. R.
Importance	Further Reading
Date	2013
Edition	
Publisher	Wiley-VCH
ISBN	9783527410699, 9783527671847
Type	Whole book
Title	Statistical mechanics: theory and molecular simulation
Authors	Tuckerman, Mark E.
Importance	Further Reading
Date	2010
Edition	
Publisher	Oxford University Press
ISBN	9780191523465, 9780198525264

Type	Whole book
Title	Understanding molecular simulation: from algorithms to applications
Authors	Frenkel, Daan, Smit, Berend
Importance	Essential Reading
Date	c2002
Edition	
Publisher	Academic Press
ISBN	9780080519982, 9780122673511, 9780122673702

Type	Whole book
Title	Computational physics
Authors	Thijssen, J. M.
Importance	Further Reading
Date	c2007
Edition	
Publisher	Cambridge University Press
ISBN	9780521833462, 9781107677135