

FYS-6306 QUANTUM THEORY OF MOLECULES AND NANOSTRUCTURES

MOLEKYyliEN JA NANORAKENTEIDEN KVANTTITEORIA

Credit units: 6 op

Lectures: 48 h

Tapio Rantala, prof.
SG219, puh. +358-40-543-3506
FirstName.LastName@tut.fi
<http://www.tut.fi/~trantala/opetus/>
--> FYS6300 ...

Exercises and demonstrations: 12 x 2 h
hossein.gholizadehkalkhoran@tut.fi
Hossein Gholizade, SG312
<http://>

Time and place: Tue 10 – 12 SG312 (Lects)
Wed 10 – 12 SG312 (Lects)
Thu 10 – 12 SG312 (Excs)

Textbook: P.W. Atkins and R.S. Friedman:
Molecular Quantum Mechanics
(5. painos); ja S.V. Gaponenko:
Optical Properties of Semiconductor Nanocrystals, Cambridge Studies in Modern Optics

In Finnish: Luentomateriaali vuodelta 2013:
<http://www.tut.fi/~trantala/opetus>

Prerequisites: Basics of physics and chemistry

Examinations: 9.12.15 (11.2.16 and 7.4.16)

SCHEDULE 2015

	WEEK	Lecture	Exercise	Note!
I August	35	Tue 1 – 2		
		Wed 3 – 4	Thu	
	36	Tue 5 – 6		
		Wed 7 – 8	Thu 1	
September	37	Tue 9 – 10		
		Wed 11 – 12	Thu 2	
	38	Tue 13 – 14		
		Wed 15 – 16	Thu 3	
	39	Tue 17 – 18		
		Wed 19 – 20	Thu 4	
I	40	Tue 21 – 22		
		Wed 23 – 24	Thu 5	
	41	Tue		
		Wed	Thu 6	
October	42			Exam week
	43	Tue 25 – 26		
		Wed 27 – 28	Thu	
	44	Tue 29 – 30		
		Wed 31 – 32	Thu 7	
I	45	Tue 33 – 34		
		Wed 35 – 36	Thu 8	
November	46	Tue 37 – 38		
		Wed 39 – 40	Thu 9	
	47	Tue 41 – 42		
		Wed 43 – 44	Thu 10	
	48	Tue 45 – 46		
		Wed 47 – 48	Thu 11	
December	49	Tue		
		Wed	Thu 12	
	50			Exam week
		Wed Exam 9.12.		
	51			Exam

CONTENTS

Introduction and orientation

1. Foundations of quantum mechanics

Operators in quantum mechanics
Postulates of quantum mechanics
Specification and evolution of states

2. Linear motion and harmonic oscillator

Characteristics of wavefunction
Translational motion
Penetration into and through barriers
Particle in a box
Harmonic oscillator
Further information

3. Rotational motion and hydrogen atom

Particle on a ring
Particle on a sphere
Motion in a Coulombic field
Further information

4. Angular momentum

Angular momentum operators
Definition of states
Angular momentum of composite systems

5. Group theory

Symmetries of objects
Calculus of symmetry
Reduced representations
Symmetry properties of functions
Full rotational groups
Applications

6. Techniques of approximation

Semiclassical approximation
Time-independent perturbation theory
Variation theory
Hellmann–Feynman theorem
Time-dependent perturbation theory
Further information

7. Atomic spectra and atomic structure

Spectrum of atomic hydrogen
Structure of helium
Many-electron atoms
Atoms in external fields

8. Introduction to molecular structure

Born–Oppenheimer approximation
Molecular orbital theory
Polyatomic molecules
Band theory of solids

9. Computational chemistry

Hartree–Fock SCF method
Electron correlation
Density functional theory (DFT)
Local-density approximation (LDA)
"Evolution of Quantum Theory" and other issues

21. Electron states in crystal

21.1. A few elementary models
21.2. Electrons in three dimensional crystal
21.3. Quasiparticles
21.4. Low-dimensional structures

22. Electrons in ideal nanocrystal

22.1. From crystal to cluster
22.2. From molecule to crystal
22.3. Size regimes
About "self-assembly of nano-scale structures"

LITERATURE

P.W. Atkins, R.S. Friedman:
Molecular Quantum Mechanics
 (Oxford University Press, Oxford, New York, 5th ed. 2011)

M. Weissbluth:
Atoms and Molecules
 (Academic Press, New York, 1983)

R.G. Parr and W. Yang:
Density-Functional Theory of Atoms and Molecules
 (Oxford University Press, Oxford, New York, 1989)

T.T. Rantala:
*Local-Density Electronic Structure Calculations
 on the Spectra and Reactivity of Metals*
 Acta Univ. Ouluensis A 184 (1987)

Jean-Louis Calais:
Quantum Chemistry Workbook
 (John Wiley & Sons, New York, 1994)

I. Lindgren och S. Svanberg:
Atomfysik
 (Universitetsförlaget Uppsala, LiberTryck Stockholm, 1974)

A. Hinchliffe:
Computational Quantum Chemistry
 (John Wiley & Sons, Chichester, New York, 1989)

S.V. Gaponenko:
Optical Properties of Semiconductor Nanocrystals
 Cambridge Studies in Modern Optics
 (Cambridge University Press, Cambridge, 1998)