Schema KZ4012 Kemisk bindning, 5 hp

HT2020 (03.12.2020 – 22.12.2020)

dag vecka	måndag	tisdag	onsdag	torsdag	fredag
49 30/11-04/12				F1 Math/RÖ1	F2 RÖ2
50 07/12-11/12	F3 RÖ3	F4 La1**A**|RÖ4**B**	F5 RÖ4**A**|La1**B**	La2**A** La2**A**	La2**B** La2**B**
51 14/12- 18/01	F6 RÖ5	F7 RÖ6	F8 RÖ7	Lab3**A** Lab3**A**	Lab3**B** Lab3**B**
52 21/12- 25/12	Reservlabb och avslut rapport skrivning	Reservlabb och avslut rapport skrivning			
01 04/01-08/01	Tenta 10-15.00				

Tider: fm 9:15 – 12; em: 13 – 16 för RÖ och 13 – 17 för labbar
F (1-8) föreläsningar, RÖ (1-7) räkneövningar, L (1-3) labbar
F1-3, F5-8: Ulrich Häussermann (ulrich.haussermann@mmk.su.se)
F4: Paulo Barros (paulo.barros@mmk.su.se)
Math Paulo Barros (paulo.barros@mmk.su.se
RÖ1-3: Paulo Barros (paulo.barros@mmk.su.se),
RÖ4-7 Ulrich Häussermann (ulrich.haussermann@mmk.su.se
Labb 1 – 3: Paulo Barros (paulo.barros@mmk.su.se)

Plats: Sal **K441-447** för tenta, föreläsningar och övningar (zoom och in person om man vill, max 10 personer). Datasalen för labbarna (La1-3, på plats. Grupp **A** och **B**, max 10 peroner per grupp).

Kurslitteratur:

1) P. Atkins, J. de Paula, R. Friedman, "Quanta, Matter and Change", Second edition, Oxford, 2014; (används tidigare i fysikalisk kemi)
2) "Inorganic Chemistry" 7th edition , 2018 (by Mark Weller, Tina Overton, Jonathan Rourke, Fraser Armstrong) ISBN: 9780198768128 (används senare i oorganisk kemi), Kapitel 1, 2, 3.

Föreläsningar (focus & topic info refer to the Atkins book)

F1 – F4: Molecular structure (Focus 6)

F1: Repetition H-atom and many-electron atoms (topics 18, 19), periodicity (topic 20), atomic spectroscopy (brief) (topic 21). Outlook molecules.

F2: Molecular orbital theory, effective Hamiltonians, variation principle (topic 23), homonuclear and heteronuclear diatomic molecules, the polar bond (topics 24, 25),

F3: Polyatomic molecules, π-systems and Hückel approach (topic 26), valence bond theory (topic 22)

F4: Introduction into Gaussian program package (used in the computer lab), self consistent fields (topic 27), ab-inito methods and DFT (excerpts topics 29, 30), examples of computational chemistry

F5 – F7: Molecular symmetry (Focus 7)

F5: Symmetry in chemistry, analysis of molecular shape, symmetry elements and operations, symmetry classification of molecules (topic 31)

F6: Group theory and its tools (topic 32), applications of symmetry (topic 33)

F7: Application of symmetry to orbitals: revisit ring systems (organic molecules), MOs for basic shapes of inorganic molecules, symmetry adaption of ligand basis functions, valence bond theory vs MO theory

F8: Vibrational and electronic spectroscopy (Focus 9)

F8: Vibrational spectroscopy of polyatomic molecules: IR and Raman spectrometers (topic 40, excerpts), normal modes, selection rules, interpretation of spectra (topic 44), utilizing spectroscopy for the characterization of molecules. Application of symmetry to vibrational and electronic spectroscopy: irreducible representation of modes, establishing modes for basic shapes of inorganic molecules, principles of UV-VIS (absorption)spectrometers (topic 40, excerpts), electronic spectroscopy, electronic transitions (topic 45).

F9: Q&A, Exam preparation (frågestund…).

Räkneövningar:

Math: introduction/repetition of some linear algebra (linear equation systems, matrices, determinants)

RÖ1: Properties of atomic orbitals, construction of diatomic MOs

RÖ2 and 3: Exercising the Hückel method (setting up hamiltonian matrices and diagonalization): allyl system, butadien system, general ring systems (e.g. benzene and cyclopentadiene. By hand and with Matlab.

RÖ4: Finding symmetry elements, handling symmetry operations, symmetry classification of molecules.

RÖ5: Application of symmetry to orbitals, part1

RÖ6: Application of symmetry to orbitals, part 2

RÖ7: Application of symmetry to vibrations

Laboratory:

1. Computer-lab 1: Atoms and diatomic molecules (homo- and heteronuclear) O_2, LiF. MO diagrams, potential energy curves, dissociation energy.

2. Computer-lab2: Polyatomic molecules. AH_2 (BeH_2, OH_2). Walsh diagram, number of valence electrons governs molecular structure. Organic molecules (isomers of butadiene). Geometry optimization, determination of most stable isomers from Gaussian calculations.

3. Spectroscopy-lab: Calculation of vibrational frequencies of polyatomic molecules, collecting Raman, IR, UV-VIS spectra of various compounds. Evaluation and interpretation of spectroscopic data.