UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	MOLEKULSKO MODELIRANJE
Course Title:	MOLECULAR MODELLING

Študijski program in stopnja Study Programme and Level	Študijska smer Study Field	Letnik Academic Year	Semester Semester
MAG Kemija, 2. stopnja	**/**	**2.**	**3.**
USP Chemistry, 2nd Cycle	**/**	**2nd**	**3rd**

Vrsta predmeta / Course Type: obvezni / Mandatory

Univerzitetna koda predmeta / University Course Code: KE221

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
45	**/**	**30 LV**	**/**	**/**	**/**	**5**

Nosilec predmeta / Lecturer: prof. dr. Barbara Hribar Lee / dr. Barbara Hribar Lee, Full Professor
doc. dr. Črtomir Podlipnik / dr. Črtomir Podlipnik, Assistant Professor

Jeziki / Languages:

Predavanja / Lectures:	**slovenski / Slovenian**
Vaje / Tutorial:	**slovenski / Slovenian**

Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:	Prerequisites:
Študent oz. kandidat mora imeti predmet opredeljen kot študijsko obveznost.	The course has to be assigned to the student.

Vsebina:	Content (Syllabus outline):
Ponovitev osnov kvantne mehanike ter fizike atomov in molekul (Schrödingerjev in Heisenbergov pristop, Schrödingerjeva enačba, Paulijev izključitveni princip). Opis in reševanje modelnih primerov: delec in pregrade, togi rotator, harmonski oscilator, vodikov atom. Metode za približno računanje: variacijska metoda in metoda motenj. Modeli za obravnavanje molekulskih sistemov: teorija valenčnih vezi in teorija molekulskih orbital, Hartree-Fockov model. Pregled metod, sistemov in ciljev modeliranja. Elektronska struktura: ab initio, semiempirične metode, gostotni funkcionali. Molekulska mehanika, molekulska dinamika, Monte Carlo.	Recurrence of the basics of quantum mechanics of atoms and molecules (Schrödinger's and Heisenberg's approach, Schrödinger equation, Pauli exclusion principle). Description of basic quantum mechanical models and principles, solving various relevant problems as such as particle in potential box, rigid rotor, harmonic oscilator, hydrogen atom. Methods for approximative computations: the variational principle and perturbation theory. Modelling of molecular systems: valence bond theory and molecular orbital theory, Hartre-Fock model. Review of methods, systems and objectives of molecular modeling. Molecular electronic structure: ab initio and semiempirical methods,

Pomen in uporaba grafike pri modeliranju. Skupine sistemov, primerne za modeliranje: manjše molekule v vakuumu, vpliv okolice, interakcije med molekulami, modeliranje kemijskih reakcij (prehodna stanja), pomoč eksperimentalnim rezultatom z metodami modeliranja. Področje dela računalniške kvantne kemije, glavne metode in računski modeli, pregled pomembnih računalniških sistemov na tem področju, prikaz praktičnega dela z računalnikom na konkretnem problemu, individualno obravnavanje enostavnejših primerov s pomočjo metod kvantne kemije.	density functional theory. Force field based methods: Molecular mechanics, molecular dynamics, Monte Carlo method. Molecular graphics and its importance for molecular modeling. Systems for molecular modeling: small molecules in vaccuo, solvent effect, intra and inter-molecular interactions, modeling of chemical reactions (transition states). Know how to use a molecular modeling as a support of laboratory experiments. Overview of methods and computer programs for molecular modeling and/or quantum chemical computations. Practical work with the computer on relevant problems from the field of molecular modeling and/or quantum chemistry.

Temeljna literatura in viri / Readings:

- A.R. Leach, Molecular Modelling, Principles and Applications, Addison Wesley Longman, London 1998, 585 str., (34 %)
- A. Hinchliffe, Molecular Modelling for Beginners, Wiley, Chichester 2003, 401 str., (50 %)

Dopolnilna literatura:

- J. Koller, Struktura atomov in molekul – osnove kvantne mehanike, atomi, FKKT, Ljubljana 2002, 117 str.
- J. Koller, Struktura atomov in molekul – molekule, osnove spektroskopije, FKKT, Ljubljana 2000, 114 str.
- Priročniki za uporabo računalniških programov

Cilji in kompetence:	**Objectives and Competences:**
Cilji modeliranja: poznavanje elektronske strukture in geometrije molekul (iz osnovnih podatkov), napoved lastnosti molekul in njihova povezava s strukturo, podobnost molekul, možnost načrtovanja molekul z vnaprej določenimi želenimi lastnostmi. *Kompetence:* razumevanje in obvladovanje vloge računalniške grafike pri molekulskem modeliranju. Pregled najbolj znanih računalniških programov za uporabo pri modeliranju (Gaussian, Spartan, HyperChem ...), prikaz praktičnega dela na osebnem računalniku, delovni postaji in velikem računalniku (preko računalniške mreže). Sistematični pregled celotne snovi.	Objectives: The knowledge (prediction) of molecular geometry and molecular electronic structure. The use of molecular modeling and quantum mechanical methods for prediction of molecular properties. Qualitative and quantitative structure-property relationships. Structure based design of molecules with certain properties. Competences: Overview of well-known programs for molecular modeling and quantum chemical computations as such as Gaussian, Spartan, HyperChem, Schrodinger Suite with hands on sessions on personal comuterm working station and big cluster (using web interface).

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
Znanje in razumevanje Predmet je namenjen nadgradnji znanja kvantne kemije in njeni praktični uporabi. Študente seznani s pojmom molekulskega modeliranja, ki je že dalj časa močno orodje za pomoč eksperimentalistom, saj omogoča vpogled na nekatera eksperimentom nedostopna področja znanosti. Ob koncu so sposobni formulirati problem, izbrati primerno metodo modeliranja in kritično ovrednotiti dobljene rezultate. Pomembno je potem tudi iskanje korespondence med dobljenimi teoretičnimi in v literaturi poiskanimi rezultati.	Knowledge and Comprehension This course is designed to upgrade the knowledge of quantum chemistry and its practical application. During this course the students will be introduced with molecular modeling methods and principles. Molecular modeling became an excellent toll that serve as support to experimentalist for better understanding fundamental and applicative science. At the end of the course students will be able to formulate problem, to select and to set up a proper molecular modeling method, and also to evaluate obtained results critically. They will be also able to compare the experimental data either from literature and/or laboratory with the data resulted from computional chemistry approach.
Uporaba Slušatelj je sposoben uporabiti znanje kvantne kemije za modeliranje danega kemijskega ali biokemijskega problema, komercialne računalniške programske sisteme s tega področja mu ni več potrebno uporabljati kot "black box", zaradi česar lahko tudi mnogo bolj kompetentno razlaga dobljene rezultate.	Application The student is able to use quantum chemistry knowledge for modeling of certain chemistry orbiochemistry problem. The background that the student obtains in the course transforms her/him into an advanced user of computational chemistry software. They are able to competently interpret computational chemistry results.
Refleksija Študent si pridobi občutek, da se lahko v primeru nepremostljivih eksperimentalnih težav še vedno zateče k računu, kjer so problemi drugačni in navadno drugje, kar pogosto privede do zadovoljive razjasnitve problema.	Analysis The information from the computational experiment are often complementary than those obtained from laboratory experiment. The proper combination of laboratory and computational work often leads to more relevant description of the problem.
Prenosljive spretnosti Pri predmetu se študenti naučijo prepoznavati problem, ga prevesti v matematično obliko, rešiti in na koncu interpretirati rezultate. Poseben poudarek je na kritičnem ovrednotenju dobljenih rezultatov. Naučijo se uporabe domače in tuje literature ter podajanja zaključenega dela v pisni obliki.	Skill-transference Ability In this course the students are able to recognize a problem, to transform it to mathematical form, to solve the problem and at the end to interpret results. The critical evaluation of the results is one of the most important skills that students learn during the course. At the end of the course the students learn how to write a scientific report and to perform scientific presentation.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
- Predavanja - Seminar (računske naloge iz predelane snovi) - Praktične vaje na računalniku	- Lectures - Seminars - Laboratory Lessons (Using computer)

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Ustni izpit Seminarska naloga Ocene: 6-10 (pozitivno).	**60 %** **40 %**	Oral exam Seminar

Reference nosilca / Lecturer's references:

prof.dr.Barbara Hribar Lee:
- M. Luksic, T. Urbic, B. Hribar-Lee, K. A. Dill, Simple Model of Hydrophobic Hydration, J. Phys. Chem. B, 2012, 116 (21), 6177– 6186.
- B. Hribar-Lee, K. A. Dill, V. Vlachy, Receptacle Model of Salting- In by Tetramethylammonium Ions, J. Phys. Chem. B, 2010, 114 (46), pp 15085–15091.
- K. A. Dill, T. M. Truskett, V. Vlachy, B. Hribar-Lee, Modeling water, the hydrophobic effect, and ion solvation, Annu Rev Biophys Biomol Struct, 2005, 34, 173-199.

doc. dr. Črtomir Podlipnik:
- SKRT, Mihaela, BENEDIK, Evgen, PODLIPNIK, Črtomir, POKLAR ULRIH, Nataša. Interactions of different polyphenols with bovine serum albumin using fluorescence quenching and molecular docking. *Food chem.*. [Print ed.], 2012, vol. 135, str. 2418-2424, doi: 10.1016/j.foodchem.2012.06.114. [COBISS.SI-ID 4113784]
- MARUŠIČ, Jaka, PODLIPNIK, Črtomir, JEVŠEVAR, Simona, KUZMAN, Drago, VESNAVER, Gorazd, LAH, Jurij. Recognition of human tumor necrosis factor [alpha] (TNF-[alpha]) by therapeutic antibody fragment : energetics and structural features. *J Biol Chem*, 2012, vol. 287, no. 11, str. 8613-8620, doi: 10.1074/jbc.M111.318451. [COBISS.SI-ID 35833349]
- PODLIPNIK, Črtomir, TUTINO, Federico, BERNARDI, Anna, SENECI, Pierfausto. DFG-in and DFG-out homology models of TrkB kinase receptor : induced-fit and ensemble docking. *J. mol. graph. model.*. [Print ed.], 2010, vol. 29, no. 3, str. 309-320, doi: 10.1016/j.jmgm.2010.09.008. [COBISS.SI-ID 34621701]