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):
Osnovni pojmi v molekulskem modeliranju. Zapis molekul. Molekulska grafika. Molekulske površine. Kvantnomehanski modeli. Schrödingerjeva enačba. Večelektronski sistemi. Variacijska metoda – Hartree-Fockov sistem enačb. Roothaan-Hallove in Pople-Nesbetove enačbe. Bazne funkcije in bazni seti. Korelacijska energija – konfiguracija interakcij in Møller-Plessetova perturbacijska teorija. Semiempirične metode. Teorija gostotnega funkcionala. Molekulske lastnosti, dobljene iz valovne funkcije. Mehanski modeli – empirična polja sil. Vezne interakcije. Nevezne interakcije. Reducirana	Useful concepts in molecular modelling. Molecular file formats. Molecular graphics. Molecular surfaces. Quantum mechanical models. Schrödinger equation. Polyelectronic systems. Variation method - Hartree-Fock equations. Roothaan-Hall and Pople-Nesbet equations. Basis functions and basis sets. Correlation energy – configuration interaction and Møller – Plesset perturbation theory. Semi-empirical methods. Density functional theory. Calculating molecular properties from the wave function. Molecular mechanics – empirical force field models. Bonded interactions. Non-bonded interactions. Reduced representation. Force

reprezentacija. Modeli za opis vode. Ovrednotenje rezultatov molekulske mehanike. Energijska minimizacija. Računalniške simulacije. Zasnova računalniških simulacij. Računalniška simulacija Monte Carlo. Računalniška simulacija molekulske dinamike. Simulirano ohlajanje. Konformacijska analiza. Vaje: uporaba različnih metod molekulskega modeliranja na praktičnih primerih.	field models for water. Calculating systems properties from molecular mechanics. Energy minimisation. Computer simulations. Basic elements of computer simulations. Monte Carlo computer simulation. Molecular dynamics computer simulation. Simulated annealing. Conformational analysis. Lab work: applying the methods of molecular modelling to practical examples.

Temeljna literatura in viri / Readings:

B. Hribar-Lee, Č. Podlipnik, Molekulsko modeliranje, UL FKKT, 2019.
Dodatna literatura:
F. Jensen, Introduction to Computational Chemistry, Wiley, Hoboken, 2007.
A. Szabo, N. S. Ostlund, Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory, Dover, New York, 1996. (10%)
A. R. Leach, Molecular Modelling, Principles and Applications, Addison Wesley Longman, London, 1998.

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:**
Pisni izpit	**50 %**	Written exam
Seminarska naloga	**50 %**	Seminar
Ocene: 6 – 10 (pozitivno)		

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]