UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	TEORETIČNE METODE V FIZIKALNI KEMIJI
Course Title:	THEORETICAL METHODS IN PHYSICAL CHEMISTRY

Študijski program in stopnja Study Programme and Level	Študijska smer Study Field	Letnik Academic Year	Semester Semester
DR Kemijske znanosti, 3. stopnja	**/**	**1.**	**1. in 2.**
Doctoral programme in Chemical Sciences, 3rd Cycle	**/**	**1st**	**1st and 2nd**

Vrsta predmeta / Course Type: izbirni/Elective

Univerzitetna koda predmeta / University Course Code: KZ307

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
30		**LV / SV**		**90**	**30**	**5**

Nosilec predmeta / Lecturer: prof. dr. Barbara Hribar Lee /Dr. Barbara Hribar Lee, Full Professor

Jeziki / Languages:

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

Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:

Študent oz. kandidat mora imeti predmet opredeljen kot študijsko obveznost.

Prerequisites:

The course has to be assigned to the student.

Vsebina:

Študent skupaj z mentorjem, izmed spodaj navedenih, izbere vsebine v obsegu 5 KT. Če je izvajalcev več, nosilec predmeta skladno z izbranimi vsebinami kooordinira izvajanje.

- *Potencialne teorije.* Osnove, Poisson−Boltzmannova enačba, modificirana Poisson−Boltzmannova enačba. Robni pogoji in rešitve linearizirane in nelinearizirane oblike v različnih simetrijah.
- *Termodinamične perturbacijske teorije.* Osnove, Gibbs−Bogoljubova neenakost. Barker−Hendersonova teorija. Weeks–

Content (Syllabus outline):

From the topics listed below, the student selects (in agreement with his supervisor) those being of most relevance for his PhD Thesis. The number of chosen hours of study must carry 5 credits. The Lecturer coordinates the process, if more than one teacher is involved.
- *Potential theories.* Basic facts. Poisson−Boltzmann equation, modified Poisson−Boltzmann equation. Boundary conditions and solution of linearized and non-linearized equation in different symmetries.
- *Thermodynamic perturbation theory.* Basics, Gibbs−Bogoliubov inequality. Barker−Henderson theory. Weeks–Chandler–

Chandler–Andersenova teorija. Wertheimova perturbacijska teorija. - *Porazdelitvene funkcije.* Ornstein–Zernikova integralska enačba v različnih približkih. Razvoj po multipolih za molekularne sisteme. Wertheimova integralska enačba za sisteme z usmerjenimi silami. - *Simulacijske metode.* Metoda Monte Carlo v generaliziranem ansamblu. Uporaba adhezivnega (impulznega) potenciala za modeliranje privlačnih koloidov. Dinamika molekul. Polje sil. Molekulsko prileganje (docking). Simulacije biomolekul. - *Sistemi v polju zunanje sile.* Teorija gostotnega funkcionala. - *Kvantno-kemijske metode.* Periodični sistemi: Blochove funkcije, Hartree-Fockova metoda za periodične sisteme. Korelirano gibanje elektronov: korelacijska energija, metoda konfiguracijske interakcije, multi-konfiguracijska interakcija, metoda sklopljenih skupkov. Teorija gostotnih funkcionalov (DFT): Kohn-Shamove enačbe, Hohenberg-Kohnova teorema, lokalni približek, globalni približek. Metode kvantne dinamike in mehanike. - *Kemijska kinetika.* Hitrost kemijskih reakcij v raztopinah. Vpliv ionskih reaktantov. Kataliza.	Andersen theory. Wertheim's thermodynamic perturbation theory. - *Distribution functions.* Ornstein–Zernike integral equation in different closures. Multipole expansion for molecular systems. Wertheim's integral equations for systems with highly directional forces. - *Simulation methods.* Monte Carlo method in generalized ensemble. Use of impulse potential for modelling of attractive colloids. Molecular dynamics. Force fields. Molecular docking. Simulation of biomolecules. - *Systems in external fields.* Density functional theory. - *Quantum chemistry methods.* Periodical systems: Bloch functions, Hartree-Fock method for periodical systems. Correlation in electron motion: correlation energy, method of configuration interaction, multi-configuration interaction, coupled cluster method. Density functional theory (DFT): Kohn-Sham equations, Hohenberg-Kohn theorems, local approximations, non-local approximations. Methods of quantum dynamics and mechanics. - *Chemical kinetics.* Rate of chemical reaction in solutions and effects of ionic reactants on the reaction rate. Catalysis.

Temeljna literatura in viri / Readings:

Aktualni članki iz področja predmeta. / Current literature from the field and papers related with student's research work.

Cilji in kompetence:	**Objectives and Competences:**
Naloga statistične termodinamike je, da iz podatkov o lastnostih atomov in molekul ter sil med njimi izpelje makroskopske lastnosti snovi. Drugače povedano, veda omogoča interpretacijo merskih rezultatov na molekularnem nivoju.	The purpose of statistical thermodynamics is to predict macroscopic properties of thermodynamic systems, using as input the knowledge about constituent atoms (or molecules) and forces between them. This knowledge makes it possible to interpret experiments on the molecular level.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
<u>Znanje in razumevanje</u> Poznavanje osnov statistične termodinamike, ki jih obravnava ta predmet, omogoča globlje razumevanje pojmov iz osnovne fizikalne kemije ter interpretacijo eksperimentalnih podatkov na osnovi lastnosti atomov in molekul.	<u>Knowledge and Comprehension</u> Basic knowledge of statistical thermodynamics enables the students to acquire a deeper understanding of the physical chemistry concepts, allowing interpretations of the experimental data in view of the properties of atoms and molecules.

Uporaba Študent spozna moderne računske metode za študij lastnosti snovi. Metode se uporabljajo v kemiji, farmaciji in biologiji pa tudi pri načrtovanju različnih tehnoloških procesov kot so, na primer, separacijske metode. Predmet je osnova teoretičnemu raziskovalnemu delu na področju kemije in kemijskega inženirstva.	Application The students learn modern computational methods, used for studying the properties of different substances. The methods are used in chemistry, pharmacy and biology, as well as in planning different technological processes, such as separation methods. The course is providing theoretical basis for research work in the field of chemistry and chemical engineering.
Refleksija Znanje, ki si ga pridobi student ob temu predmetu, omogoča kritično analizo merskih podatkov in je osnova za razumevanje merljivih makroskopskih količin in njihovih soodvisnosti.	Analysis The knowledge that the students obtain during this course allows critical assessment of measuring data and forms the basis for understanding of measurable macroscopic quantities and their correlations.
Prenosljive spretnosti Spretnost uporabe domače in tuje literature in drugih virov, identifikacija in reševanje problemov, postavljanje fizikalnih modelov, kritična analiza rezultatov, kvantitativno razumevanje drugih (bolj opisnih) predmetov. Nauči se numeričnega programiranja in spozna komercialne programske pakete za reševanje različnih numeričnih problemov.	Skill-transference Ability The ability of using different literature, as well as other resources, identification and problem solving, modeling of physical phenomena, critical evaluation of the results, quantitative interpretation of knowledge obtained in other courses. Students learn numerical programming and get familiar with commercial program packages for solving different numerical problems.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predavanja, samostojni študij relevantnih člankov in diskusija v skupini.	Lectures. Study of the relevant scientific literature and discussion in the research group.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Način preverjanja znanja se dogovori individualno z vsakim študentom doktorskega študija in se lahko izvaja v obliki ustnega in/ali pisnega izpita, seminarja ali izdelave projekta oziroma pisanja znanstvenega članka.	100 %	The assessment method is chosen individually and can be in the form of an oral and/or written exam, a seminar work, a project work, or writing the scientific article.

Reference nosilca / Lecturer's references:

- MOHORIČ, Tomaž, URBIČ, Tomaž, HRIBAR-LEE, Barbara. The application of the integral equation theory to study the hydrophobic interaction. *The Journal of chemical physics*, 2014, vol. 140, no. 2, art. no. 024502.
- HRIBAR-LEE, Barbara, PIZIO, Orest. Density anomaly of charged hard spheres of different diameters in a mixture with core-softened model solvent. Monte Carlo simulation results. *Condensed matter physics*, 2013, vol. 16, no. 4, art. no. 43607.

- MOHORIČ, Tomaž, URBIČ, Tomaž, HRIBAR-LEE, Barbara. The application of the thermodynamic perturbation theory to study the hydrophobic hydration. *The Journal of chemical physics*, 2013, vol. 139, no. 2, art. no. 024101.
- HRIBAR-LEE, Barbara. The application of the replica Ornstein-Zernike methodology for studying ionic membrane equilibria. *Acta chimica slovenica*, 2012, vol. 59, no. 3, str. 528-535.