załącznik do Regulaminu programu „visiting professor”

Osoba zgłaszająca z PW	
Tytuł i stopień naukowy	Prof. dr hab. inż.
Imię i nazwisko	Halina Szatyłowicz
Wydział	Wydział Chemiczny
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The person proposed as a visiting professor	
Title and degree	Professor Dr.
Name and surname	C. (Célia) Fonseca Guerra
Exact affiliation	Vrije Universiteit Amsterdam
E-mail address	c.fonsecaguerra@vu.nl
Description of achievements (1/2-1 page)	Célia Fonseca Guerra is professor at Vrije Universiteit Amsterdam (VU), where she heads the Supramolecular Quantum Biochemistry group, which is part of the Division of Theoretical Chemistry. She is internationally recognized for her work on hydrogen bonding, DNA and supramolecular chemistry. This has led to a membership of the Scientific Advisory Board of the Institut de Química Computational i Catàlisi at the University of Girona, Spain (2017-2022) as well as being awarded European Union Visiting Professor at Warsaw University of Technology (2013). For her excellent research, Fonseca Guerra has been awarded an NWO Aspasia grant as well as the Westerdijk Talent scheme to be promoted to full professor. In 2022, she was furthermore elected as Chemistry Europe Fellow and she was member of the core team of the Dutch Chemistry council.

Code of the course	4606-VP-ES-00010	Name of the course	Polish	Zaawansowane Modelowanie Molekularne
			English	**Advanced Molecular Modeling**
Type of the course	Specialty subject/~~researcher's workshop~~			
Course coordinator	C. Fonseca Guerra		Course teacher	C. Fonseca Guerra
Implementing unit	Faculty of Chemistry WUT	Scientific discipline / disciplines*	chemical sciences, chemical engineering, materials engineering	
Level of education	Doctoral Schools	Semester	5 May 2025 till 30 May 2025	

Language of the course	English				
Type of assessment	Pass	Number of hours in a semester	30	ECTS credits	3
Minimum number of participants	10	Maximum number of participants	30	Available for students (BSc, MSc)	Yes

Type of classes		Lecture	Auditory classes	Project classes	Laboratory	Seminar
Number of hours	in a week					
	in a semester	10		10	10	

* does not apply to the Researcher's Workshop

1. Prerequisites

1st year of a Bachelor Program in Chemistry completed

2. Course objectives

Theoretical Chemistry is an integral part of modern chemistry. Many properties can be computed with chemical accuracy, which enables one to study and predict quantities that are hardly or not at all accessible using experimental techniques. Furthermore, theoretical chemistry can be used as a predictive tool to design better experiments. To design new chemical syntheses, catalysts, or pharmacologically active molecules in a more rational fashion (*i.e.*, instead of using a trial-and-error approach), it is necessary to combine accuracy with solid and profound insights into the underlying mechanisms of the electronic structure. The most useful insight is obtained through detailed analyses of the computed wavefunction and bond energy.

The goal is to obtain the skills required to translate (experimental) chemical problems into a computational approach that leads to a practical solution and understanding. A start will also be made with interpreting calculated results in terms of molecular orbitals and models of the electronic structure. An essential point in this course is the unifying nature of computational chemistry: The same theoretical methods serve as tools for solving various issues from all areas of chemistry, from theoretical and physical chemistry, via (in)organic chemistry and catalysis, to pharmaco- and biochemistry.

We will make the step from describing and understanding to rational design. This requires both a solid understanding of the physical factors behind structure and reactivity (taught in the interactive theory classes) but also expert experience in using and steering state-of-the-art software packages (trained and optimized in the hands-on computer labs).

3. Course content (separate for each type of classes)

Lecture

Interactive theory lectures in the 1st week of the course (5 May 2025 till 9 May 2025), all on location in Warsaw.

L1 – Understanding Guanine Quadruplexes with Kohn-Sham Molecular Orbital Theory

L2 – Cooperativity proves Covalency in Hydrogen Bonds and Halogen Bonds

L3 – Understanding Self-assembly in Supramolecular Chemistry:

L4 – Revealing the role of the Chalcogen atom in Supramolecular Chemistry with computational analysis tools.

L5 – Understanding donor-acceptor interactions: Metallophilic Interactions and Lewis Acid/Base Interactions.

Laboratory

This will be done in the Molecular Modelling course.

Project classes
The project classes will take place in week 2, 3 and 4 of the course Advanced Molecular Modeling (12 May 2025 till 30 May 2025), and are online. They will be based on topics that we offer, and which can be adapted, in consultation between students and teacher, to specific interests of the students. The topics range from trends in structure and stability in biochemistry and supramolecular chemistry.

4. Learning outcomes

Type of learning outcomes	Learning outcomes description	Reference to the learning outcomes of the WUT DS	Learning outcomes verification methods*
Knowledge			
K01	global achievements covering theoretical foundations and general issues, as well as selected detailed issues – appropriate to the represented scientific discipline	SD_W1	final presentation & discussion
K02	the main development trends of the represented scientific discipline with the related research methodology	SD_W2	final presentation & discussion
Skills			
S01	perform critical analysis and evaluation of the results of research, expert works, and other creative activities, as well as their contribution to the development of knowledge, in particular - evaluate usefulness and the ways to use the results of theoretical works in practice	SD_U1	final presentation & discussion
Social competences			
SC01	recognizes the importance of knowledge and academic achievements in solving cognitive and practical problems	SD_K1	final presentation & discussion

*Allowed learning outcomes verification methods: exam; oral exam; oral test; project evaluation; report evaluation; presentation evaluation; active participation during classes; homework; tests

5. Assessment criteria

Assessment is based on the combined evaluation of the interactive classroom participation + the final presentations of the research projects. The grades that can be obtained are: FAIL, or PASS, or EXCELLENT.

6. Literature

Primary references:

[1] Telomere Structure and Stability: Covalency in Hydrogen Bonds, Not Resonance Assistance, Causes Cooperativity in Guanine Quartets. C. Fonseca Guerra, H. Zijlstra, G. Paragi, F. M. Bickelhaupt. *Chem. Eur. J.* 2011, 17, 12612-12622

[2] The Role of Alkali Metal Cations in the Stabilization of Guanine Quadruplexes: Why K+ is the best. F. Zaccaria, G. Paragi, C. Fonseca Guerra, *Phys. Chem. Chem. Phys.* 2016, 18, 20895-20904

[3] Secondary Electrostatic Interaction Model Revised: Prediction Comes Mainly from Measuring Charge Accumulation in Hydrogen-Bonded Monomers. S. C. C. van der Lubbe, F. Zaccaria, X. Sun, C. Fonseca Guerra, *J. Am. Chem. Soc.* 2019, *141*, 4878-4885

[4] Hydrogen bond strength of CC and GG pairs is determined by steric repulsion: electrostatics and charge transfer overruled. S. C. C. van der Lubbe, C. Fonseca Guerra, *Chem. Eur. J.* 2017, *23*, 10249-10253

[5] How the Chalcogen Atom Size Dictates the Hydrogen-Bond Donor Capability of Carboxamides, Thioamides, and Selenoamides. C. Nieuwland, C. Fonseca Guerra, *Chem. Eur. J.* 2022, *28*, e202200755.

[6] Relevance of Orbital Interactions and Pauli Repulsion in the Metal-Metal Bond of Coinage Metals. M. B. Brands. J. Nitsch, C. Fonseca Guerra, *Inorg. Chem* 2018, *57*, 2603-2608.

Secondary references:

[1] Cooperativity in the Self-Assembly of the Guanine Nucleobase into Quartet and Ribbon Structures on Surfaces. G. Paragi, C. Fonseca Guerra, *Chem. Eur. J.* 2017, *23*, 3042-3050

[2] σ-Electrons Responsible for Cooperativity and Ring Equalization in Hydrogen-Bonded Supramolecular Polymers. L. de Azevedo Santos, D. Cesario, P. Vermeeren, S. C. C. van der Lubbe, F. Nunzi, C. Fonseca Guerra, *ChemPlusChem* 2022, *87*, e202100436

7. PhD student's workload necessary to achieve the learning outcomes**		
No.	Description	Number of hours
1	Hours of scheduled instruction given by the academic teacher in the classroom	30
2	Hours of consultations with the academic teacher, exams, tests, etc.	10
3	Amount of time devoted to the preparation for classes, preparation of presentations, reports, projects, homework	30
4	Amount of time devoted to the preparation for exams, test, assessments	20
	Total number of hours	**90**
	ECTS credits	**3**

** 1 ECTS = 25-30 hours of the PhD students work (2 ECTS = 60 hours; 4 ECTS = 110 hours, etc.)

8. Additional information	
Number of ECTS credits for classes requiring direct participation of academic teachers	1
Number of ECTS credits earned by a student in a practical course	2