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-00009	Name of the course	Polish	Modelowanie Molekularne
			English	**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	31 March 2025 till 25 April 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.

One purpose of this course is learning and working with state-of-the-art quantum chemical and molecular mechanical methods and computer software. For that, the students are introduced to the quantum chemical software. The goal is two-fold: 1) knowledge about the quantum chemical software, such as basis sets, numerical integration, determination of optimal geometry and transition-states, application of symmetry, use of solvation in quantum chemistry) and 2) utilization of the soft-ware code (Amsterdam Density Functional Program) to to predicting structures, exploring potential energy surfaces (e.g., for obtaining reaction profiles), and computation of molecular properties.

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

Lecture

Interactive theory lectures in the 1st week of the course (31 March 2025 till 4 April 2025), all on location in Warsaw.

L1 – Introduction to quantum chemistry (Independent Particple Model)

L2 – Quantum chemical software (Amsterdam Density Functional Program)

L3 – Atomic charges (Mulliken, Hirshfeld, VDD)

L4 – Understanding Hydrogen Bonds with Kohn-Sham Molecular Orbital Theory

L5 – Application of Quantum Chemistry in Biochemistry: DNA Replication

Laboratory

The hands-on computer labs will take place in week 2, 3 and 4 of the course (from 7 April 2025 till 25 April 2025), and are online. The labs start with a training in basic skills (installation, GUI, basic options), and continue with structural and stability exploration (including geometry optimization, vibrational analyses, spectral and other properties, Kohn-Sham MO analysis, Voronoi Deformation Density).

Project classes

This will be done in the Advanced Molecular Modelling course.

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	Exercise reports
K02	the main development trends of the represented scientific discipline with the related research methodology	SD_W2	Exercise reports
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	Exercise reports
Social competences			
SC01	recognizes the importance of knowledge and academic achievements in solving cognitive and practical problems	SD_K1	Exercise reports

*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 exercise reports. The grades that can be obtained are: FAIL, or PASS, or EXCELLENT.

6. Literature

Primary references:

[1] Voronoi Deformation Density (VDD) charges. Assessment of the Mulliken, Bader, Hirshfeld, Weinhold and VDD methods for Charge Analysis. C. Fonseca Guerra, J. -W. Handgraaf, E. J. Baerends, F. M. Bickelhaupt, *J. Comput. Chem* 2004, *25*, 189-210

[2] Chemistry with ADF. G. te Velde, F. M. Bickelhaupt, E. J. Baerends, C. Fonseca Guerra, S. J. A. van Gisbergen, J. G. Snijders, T. Ziegler, *J. Comput. Chem.* 2001, 22, 931-967

[3] Understanding Chemistry with the Symmetry-Decomposed Voronoi Deformation Density (VDD) Charge Analysis, C. Nieuwland, P. Vermeeren, F. M. Bickelhaupt, C. Fonseca Guerra, *J. Comput. Chem.* 2023, 44, 2108–2119

[4] The Nature of the Hydrogen Bond in DNA Base Pairs: the role of Charge Transfer and Resonance Assistance. C. Fonseca Guerra, F. M. Bickelhaupt, J. G. Snijders, E. J. Baerends, *Chem. Eur. J.* 1999, *5*, 3581-3594

Secondary references:

[1] Hydrogen Bonding in DNA Base Pairs: Reconciliation of Theory and Experiment. C. Fonseca Guerra, F. M. Bickelhaupt, J. G. Snijders, E. J. Baerends, *J. Am. Chem. Soc.* 2000, *122*, 4117-4128

[2] B-DNA Structure and Stability: The Role of Hydrogen Bonding, π–π Stacking Interactions, Twist-Angle, and Solvation. J. Poater, M. Swart, F. M. Bickelhaupt, C. Fonseca Guerra, *Org. Biomol. Chem.* 2014, 12, 4691-4700

[3] Selectivity in DNA Replication. Interplay of Steric Shape, Hydrogen Bonds, π-Stacking and Solvent Effects. J. Poater, M. Swart, C. Fonseca Guerra, F. M. Bickelhaupt. *Chem. Commun.* 2011, 47, 7326-7328

[4] Orbital interactions in strong and weak hydrogen bonds are essential for DNA replication. C. Fonseca Guerra, F. M. Bickelhaupt, *Angew. Chem. Int. Ed.* 2002, 41, 209

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