załącznik do Regulaminu programu „visiting professor”

Osoba zgłaszająca z PW	
Tytuł i stopień naukowy	Prof. dr hab. inż.
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The person proposed as a visiting professor	
Title and degree	Professor Dr.
Name and surname	F. M. (Matthias) Bickelhaupt
Exact affiliation	Vrije Universiteit Amsterdam
E-mail address	f.m.bickelhaupt@vu.nl
Description of achievements (1/2-1 page)	Matthias Bickelhaupt holds Chairs in Theoretical Chemistry at Vrije Universiteit (VU) Amsterdam and Radboud University Nijmegen, is Head of the VU Department of Chemistry & Pharmaceutical Sciences, and Chairman of the Holland Research School of Molecular Chemistry. Since 2022, he has been Distinguished Visiting Professor at the University of Johannesburg. Bickelhaupt is known for his work on developing theories and models of chemical bonding and reactivity, with applications in physical, (in)organic, and biological chemistry. After obtaining his Ph.D. with Nico Nibbering (UvA) and Evert Jan Baerends (VU) in 1993, he worked with Paul von Ragué Schleyer (Erlangen), Tom Ziegler (Calgary), and Roald Hoffmann (Cornell), became an assistant professor in Marburg in 1997, and obtained tenure at VU Amsterdam in 1999. Matthias Bickelhaupt received various prizes and honors, including the Dutch Research Council's VICI award, membership of the Royal Holland Society for Sciences and Humanities (KHMW), Chemistry Europe Fellow, and Member of Merit of the Royal Netherlands Chemical Society (KNCV). He has also been active in various organizational offices for science publishers (e.g., Editorial Advisory Boards) and funding agencies (e.g., ERC or NWO panels; NWO/ENW Tafel Chemie).

Code of the course	4606-VP-ES-00011	Name of the course	Polish	**Zaawansowana Chemia Obliczeniowa**
			English	**Advanced Computational Chemistry**
Type of the course	Specialty subject/~~researcher's workshop~~			
Course coordinator	F. M. Bickelhaupt	Course teacher	F. M. Bickelhaupt	
Implementing unit	Faculty of Chemistry WUT	Scientific discipline / disciplines*	chemical sciences, chemical engineering, materials engineering	
Level of education	Doctoral Schools	Semester	31 March 2025 - 25 April 2025, and 5 May 2025 - 30 May 2025	
Language of the course	English			
Type of assessment	Pass	Number of hours in a semester	60	ECTS credits: 6
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	20		15	25	

* does not apply to the Researcher's Workshop

1. Prerequisites

Students should have passed the first year of a bachelor program in chemistry.

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. In addition to the more conventional *ab initio* methods (*e.g.*, Hartree-Fock and post-Hartree-Fock theory), density functional theory (DFT) is also discussed. These are applied, for example, to predicting structures, exploring potential energy surfaces (e.g., for obtaining reaction profiles), and computation of molecular properties.

A second 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.

Last but not least, 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
The interactive theory classes comprise 10 lectures, all on location in Warsaw: 5 lectures in week 1 (31 March till 4 April 2025: L1 - L5) and 5 lectures in week 5 (5 May till 9 May 2025: L6 - L10) and address the following topics: L1: Introduction and essentials of Hartree-Fock (HF) theory L2: Essentials of Kohn-Sham density functional theory (DFT) L3: Activation Strain Model (ASM) of chemical reactivity and Energy Decomposition Analysis (EDA) L4: Paradigm shifts in chemical-bonding theory L5: Captodative effect and heavier main-group elements L6: Weak interactions L7: Aromaticity and hypervalence L8: The S_N2/E2 competition L9: Cyclo-Addition Reactions L10: Homogeneous catalysis
Laboratory
The hands-on computer labs take place in weeks 2, 3 and 4 (7 April till 25 April 2025) of the course, and are online. They start with a training in basic skills (installation, GUI, basic options), followed by structural and stability exploration (including geometry optimization, vibrational analyses, spectral and other properties, Kohn-Sham MO analysis), and finally reactivity and catalysis (determination of transition states, intrinsic reaction coordinates.
Project classes
The project classes take place in weeks 6, 7 and 8 (12 May till 30 May 2025) of the course, and are online. They are based on topics that are related to the interactive theory classes, and that 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 organic and inorganic molecules and ions, via elementary reactions in (in)organic chemistry and catalysis, to intermolecular interactions.

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	1) exercise reports 2) final presentation & discussion
K02	the main development trends of the represented scientific discipline with the related research methodology	SD_W2	1) exercise reports 2) 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	1) interactive classroom participation 2) 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 exercise reports + the final presentations of the research projects. The grades that can be obtained are: FAIL, or PASS, or EXCELLENT.

6. Literature

Primary references:

[1] **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

[2] **Analyzing Reaction Rates with the Distortion/Interaction-Activation Strain Model.** F. M. Bickelhaupt, K. N. Houk, *Angew. Chem. Int. Ed.* 2017, *56*, 10070-10086

[3] **Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry.** F. M. Bickelhaupt, E. J. Baerends In: *Reviews in Computational Chemistry*; K. B. Lipkowitz and D. B. Boyd, Eds.; Wiley-VCH: New York, 2000, Vol. 15, pp. 1-86.

[4] **Essentials of Computational Chemistry, 2nd Edition**, Christopher J. Cramer, John Wiley & Sons, 2004, ISBN 0-470-09182-7.

Secondary references:

[1] S. C. A. H. Pierrefixe, F. M. Bickelhaupt —— "Aromaticity. Molecular Orbital Picture of an Intuitive Concept" —— Chem. Eur. J. 2007, 13, 6321-6328 (Cover).

[2] S. C. A. H. Pierrefixe, C. Fonseca Guerra, F. M. Bickelhaupt —— "Hypervalent Silicon versus Carbon: Ball-in-a-Box Model" —— Chem. Eur. J. 2008, 14, 819-828 (Cover).

[3] T. Hansen, X. Sun, M. Dalla Tiezza, W.-J. van Zeist, J. N. P. van Stralen, D. P. Geerke, L. P. Wolters, J. Poater, T. A. Hamlin, F. M. Bickelhaupt —— "C–X Bond Activation by Palladium: Steric Shielding versus Steric Attraction" —— Chem. Eur. J. 2022, 28, e202201093/1-10.

[4] G. Th. de Jong, F. M. Bickelhaupt —— "Catalytic Carbon–Halogen Bond Activation. Trends in Reactivity, Selectivity and Solvation" —— J. Chem. Theory Comput. 2007, 3, 514-529.

[5] P. Vermeeren, T. Hansen, P. Jansen, M. Swart, T. A. Hamlin, F. M. Bickelhaupt —— "A Unified Framework for Understanding Nucleophilicity and Protophilicity in the SN2/E2 Competition" —— Chem. Eur. J. 2020, 26, 15538-15548.

[6] E. Blokker, W.-J. van Zeist, X. Sun, J. Poater, J. M. van der Schuur, T. A. Hamlin, F. M. Bickelhaupt —— "Methyl Substitution Destabilizes Alkyl Radicals" —— Angew. Chem. Int. Ed. 2022, 61, e202207477/1-6.

[7] P. Vermeeren, W.-J. van Zeist, T. A. Hamlin, C. Fonseca Guerra, F. M. Bickelhaupt —– "Not Carbon s–p Hybridization, but Coordination Number Determines C–H and C–C Bond Length" —– Chem. Eur. J. 2021, 27, 7074-7079.

[8] L. de Azevedo Santos, T. C. Ramalho, T. A. Hamlin, F. M. Bickelhaupt —– "Intermolecular Covalent Interactions: Nature and Directionality" —– Chem. Eur. J. 2023, 28, e202203791/1-8.

[9] T. A. Hamlin, B. J. Levandowski, A. K. Narsaria, K. N. Houk, F. M. Bickelhaupt —– "Structural Distortion of Cycloalkynes Influences Cycloaddition Rates both by Strain and Interaction Energies" —– Chem. Eur. J. 2019, 25, 6342-6348.

[10] A. K. Narsaria, T. A. Hamlin, K. Lammertsma, F. M. Bickelhaupt —– "Dual Activation of Aromatic Diels-Alder Reactions" —– Chem. Eur. J. 2019, 25, 9902-9912.

[11] D. Rodrigues Silva, E. Blokker, J. M. van der Schuur, T. A. Hamlin, F. M. Bickelhaupt —– “Nature and Strength of Group-14 A–A' Bonds" —– Chem. Sci. 2024, 15, 1648-1656.

[12] E. Blokker, M. ten Brink, J. M. van der Schuur, T. A. Hamlin, F. M. Bickelhaupt —– "Origin of the Captodative Effect: The Lone-Pair Shielded Radical" —– ChemistryEurope 2023, 1, e202300006/1-8.

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	60
2	Hours of consultations with the academic teacher, exams, tests, etc.	20
3	Amount of time devoted to the preparation for classes, preparation of presentations, reports, projects, homework	60
4	Amount of time devoted to the preparation for exams, test, assessments	40
	Total number of hours	**180**
	ECTS credits	**6**

** 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	3
Number of ECTS credits earned by a student in a practical course	3