# COURSE DESCRIPTION

## *Dynamic Combinatorial Chemistry: Principles and Applications*

Academic year **2025-2026**

**1. Programme-related data**

| | |
|---|---|
| 1.1. Higher Education Institution | Babeș-Bolyai University, Cluj-Napoca |
| 1.2. Faculty | Faculty of Chemistry and Chemical Engineering |
| 1.3. Department | Doctoral School of Chemistry |
| 1.4. Field | Chemistry |
| 1.5. Level of study | Doctoral studies |
| 1.6. Degree programme / Qualification | Doctoral studies / Doctor in Chemistry |
| 1.7. Form of education | Full-time |

**2. Course-related data**

| | | | | | |
|---|---|---|---|---|---|
| 2.1. Course title | Dynamic Combinatorial Chemistry: Principles and Applications | | | Course code | **SDC-19-05** |
| 2.2. Course coordinator | Prof. dr. Niculina Daniela Hădade | | | | |
| 2.3. Seminar coordinator | Prof. dr. Niculina Daniela Hădade | | | | |
| 2.4. Year of study | I | 2.5. Semester | II | 2.6. Type of assessment | Exam |
| 2.7. Course status | Optional | | | 2.8. Course type | Specialisation subject |

**3. Total estimated time** (hours per semester of teaching activities)

| | | | | | |
|---|---|---|---|---|---|
| 3.1. Number of hours per week | **3** | of which: 3.2. course | **2** | 3.3. seminar/ laboratory/ project | **1** |
| 3.4. Total of hours in the curriculum | 36 | of which: 3.5. course | 24 | 3.6. seminar/ laboratory | **12** |
| **Time allocation for individual study (IS) and self-taught activities (ST)** | | | | | **hours** |
| Learning from textbooks, course materials, bibliography, and notes (IS) | | | | | 50 |
| Additional research in the library, on subject-specific electronic platforms, and on-site | | | | | 90 |
| Preparing seminars/ laboratories/ projects, assignments, reports, portfolios, and essays | | | | | 65 |
| Tutoring (professional guidance) | | | | | 4 |
| Examinations | | | | | 2 |
| Other activities | | | | | 3 |
| **3.7. Total hours of individual study (IS) and self-taught activities (ST)** | | | | **214** | |
| **3.8. Total hours per semester** | | | | **250** | |
| **3.9. Number of credits** | | | | **10** | |

**4. Prerequisites** (where applicable)

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| 4.1. curriculum-related | Basic knowledge of Organic and Supramolecular Chemistry |
| 4.2 skills-related | Not applicable |

**5. Specific conditions** (where applicable)

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| 5.1. course-related | ▪ The classes will take place in a room equipped with a video projector or smart board and internet access.<br>▪ Students will have access to scientific databases.<br>▪ Active participation of students will be encouraged.<br>▪ Students are expected to attend the classes with their mobile phones turned off |
| 5.2. seminar/laboratory-related | ▪ The seminars will take place in a room equipped with a video projector or smart board and internet access. |

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|---|---|
| | ▪ Students are expected to attend the seminar with their mobile phones turned off |

**6.1. Competencies resulting from the completion of the degree programme**[1]

| **Professional competencies** | |
|---|---|
| **Competency code** | **Competency** |
| **PC1** | Advanced expertise in chemistry and doctoral-level research topics |
| **PC4** | Planning, designing, and implementing an original scientific research project, in compliance with academic ethics and integrity |
| **PC5** | Applying and developing advanced research and analytical methods; critically interpreting data and formulating innovative solutions |
| **Transversal competencies** | |
| **Competency code** | **Competency** |
| **TC2** | Advanced scientific communication in Romanian and English; collaboration in interdisciplinary and multicultural settings |
| **TC3** | Advanced digital skills for research, data analysis, and dissemination; responsible use of digital tools. |

**6.2. Learning outcomes relevant to the degree programme** (as referred to in the curriculum)[2]

| **Learning outcomes targeted by the subject** | | |
|---|---|---|
| **Competency code** | **Knowledge and comprehension** | **Specific academic skills** |
| **PC1** | Advanced and up-to-date knowledge in Dynamic Constitutional Chemistry (DCC); critical understanding of the scientific literature. | Applies and synthesizes advanced concepts/theories to formulate research hypotheses; justifies the choice of scientific approaches. |
| **PC4** | Advanced research methodologies: experimental design, modern synthesis and characterization techniques in DCC, analysis and validation; principles of research project management. | Designs, plans and implements a research project; applies quality and safety procedures and documents stages and data with full traceability. |
| **PC5** | Advanced strategies for data analysis, interpretation, and integration; evaluation of methodological limitations, reproducibility, and scientific impact. | Critically analyses complex data, estimates uncertainty and formulates conclusions; proposes methodological improvements and directions for research/innovation. |
| **TC2** | Scientific terminology and communication in Romanian and English; the structure of scientific articles and presentations; good citation practices. | Writes and presents scientific results in Romanian/English coherently; provides well-argued responses to comments and peer reviews. |
| **TC3** | Digital tools for research, citation, and data processing (databases, specialized software, reference managers); responsible use of digital resources. | Uses discipline-specific digital tools effectively; manages citations; uses digital resources responsibly in research activities. |

**7. Subject-specific learning outcomes**

| **Knowledge and comprehension** |
|---|

[1] The professional and/or transversal skills targeted by the subject for which the course description is prepared will be copied from the curriculum of the degree programme. For each competency, the complete entry, including the competency code, will be copied with the exact wording that appears in the curriculum, without any changes. If no competency is copied from either of the two categories, the row corresponding to that category is deleted from the table.

[2] The learning outcomes relevant for the degree programme and targeted by the subject for which the course description is prepared will be listed. The entries, copied without any changes from the Curriculum by subject type (Core Subject/Specialisation Subject/Complementary Subject), are listed under the corresponding competency.

| |
|---|
| 1. Defining and knowing advanced concepts, theories and models of dynamic covalent chemistry (DCC); understanding the principle of thermodynamic control, reversibility of covalent bonds and their appropriate use in professional communication. |
| 2. Using advanced knowledge in chemistry to explain and interpret dynamic covalent reactions (formation of imines, hydrazones, disulfides, boronate esters, etc.) and dynamic combinatorial libraries |
| 3. Developing the ability to design and analyze systems based on dynamic covalent chemistry: macrocycles, organic molecular cages, dynamic polymers and self-healing materials. |
| 4. Understanding and applying concepts of orthogonal reactions, self-sorting and molecular machines based on DCC. |
| 5. Advanced knowledge about emerging applications of DCC in biotechnology, organic electronics, gas capture and materials science. |
| **Specific academic skills** |
| 1. The ability to integrate and correlate data from literature for the characterisation and evaluation of CCD-based systems |
| 2. Executing required tasks according to specified requirements and within imposed deadlines, respecting professional ethics and moral conduct norms. |
| 3. Solving required tasks in accordance with general objectives established through integration within a working group. |
| 4. Ability to prepare written reports and to publicly present these reports |
| 5. Improving professional activity results through involvement in activities carried out. |

**8. Contents**

| **8.1. Course** | **Teaching and learning methods** | **Remarks[3]** |
|---|---|---|
| 8.1,1. Introduction to dynamic covalent chemistry (DCC). Importance of DCC. Basic concepts: thermodynamic control, reversibility, self-correction. Criteria for reversible systems. | Interactive lecture, multimedia presentation, discussion | 2 h/weak |
| 8.1.2. The dynamic covalent bond. Requirements for dynamic covalent bonds. Catalysis of exchange, halting equilibration, exchange symmetry. Methods to confirm reversibility. | Interactive lecture, multimedia presentation, discussion | 2 h/weak |
| 8.1.3. Polar dynamic covalent reactions – C–N and C–C bonds. Formation and exchange of imines, hydrazones, oximes. Reversible aldol condensation, Knoevenagel reaction. | Interactive lecture, multimedia presentation, discussion | 2 h/weak |
| 8.1.4. Polar dynamic covalent reactions – C–O, C–S, S–S, B–O bonds. Boronic esters, thioesters, disulfides, diselenides. Dynamic pericyclic and radical reactions. | Interactive lecture, multimedia presentation, discussion | 2 h/weak |
| 8.1.5. Dynamic combinatorial libraries – Fundamentals. History and terminology of DCLs. Theoretical considerations. Template-controlled DCLs: receptors for small molecules and ions. | Interactive lecture, multimedia presentation, discussion | 2 h/weak |
| 8.1.6. Dynamic combinatorial libraries – Applications. Ligands for biomolecules. Catalysis. Self-templating and replicators. Controlling DCLs by physical means. | Interactive lecture, multimedia presentation, discussion | 2 h/weak |
| 8.1.7. Shape-persistent macrocycles through dynamic covalent reactions. Thermodynamic vs. kinetic approach. | Interactive lecture, multimedia presentation, discussion | 2 h/weak |

[3] For example, organisational aspects, recommendations for students, specific aspects relating to the course/seminar, such as inviting experts in the field, etc.

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| Macrocycles through alkyne, imine, and olefin metathesis. | | |
| 8.1.8. Organic molecular cages (OMCs) through dynamic covalent reactions. Synthesis of OMCs through imine reaction, boronic acid condensation. Functionalization and applications of OMCs. | Interactive lecture, multimedia presentation, discussion | 2 h/weak |
| 8.1.9. Orthogonal dynamic covalent reactions. Combining orthogonal DCC reactions: imine-disulfide, imine-boronate ester. DCvC and hydrogen bonding, π-stacking interactions. | Interactive lecture, multimedia presentation, discussion | 2 h/weak |
| 8.1.10. Self-sorting through dynamic covalent chemistry and synthetic molecular machines. Thermodynamic vs. kinetic control of self-sorting. Molecular shuttles, motors, molecular walkers. | Interactive lecture, multimedia presentation, discussion | 2 h/weak |
| 8.1.11. Responsive dynamic covalent polymers and self-healing polymers. Thermoresponsive, photoresponsive, mechanoresponsive, pH-responsive polymers. Self-healing mechanisms through DCC. | Interactive lecture, multimedia presentation, discussion | 2 h/weak |
| 8.1.12. Emerging applications of dynamic covalent chemistry. Rearrangeable polymer networks. Biotechnological applications. Organic electronics, gas capture, catalysis, molecular separations. Perspectives. | Interactive lecture, multimedia presentation, discussion | 2 h/weak |

Bibliography:


1. Dynamic Covalent Chemistry: Principles, Reactions, and Applications, W. Zhang, Y. Jin, , John Wiley & Sons, Chichester, 2018.
2. Dynamic Combinatorial Chemistry Directed by Proteins and Nucleic Acids. M. Kieffer, J. F. Miron, J. G. Rudick, *Chem. Soc. Rev.* 2025, 54, 1234–1290.
3. Constitutional Dynamic Selection at Low Reynolds Number in a Triple Dynamic System: Covalent Dynamic Adaptation Driven by Double Supramolecular Self-Assembly. J. Rubio-Merino, J.-M. Lehn,* *J. Am. Chem. Soc.* 2021, 143, 15050–15063.
4. Smart Healable Polyurethanes: Sustainable Problem Solvers Based on Constitutional Dynamic Chemistry. X. Zhou, L. Zhang, Y. Chen, *Mater. Chem. Front.* 2023, 7, 3200–3235
5. Naphthalenediimide – A Unique Motif in Macrocyclic and Interlocked Supramolecular Structures. A. Diac, M. Matache, I. Grosu. N. D. Hădade,***** *Adv. Synth. Catal*. **2018**, *360*, 817–845
6. Selective Host Molecules Obtained by Dynamic Adaptive Chemistry. M. Matache, E. Bogdan, N. D. Hădade,* *Chem. Eur. J.* **2014**, *20*, 2106–2131.
7. From Supramolecular Chemistry Towards Constitutional Dynamic Chemistry and Adaptive Chemistry. J.-M. Lehn, *Chem. Soc. Rev.* 2007, 36, 151–160.


| **8.2. Seminar/ laboratory** | **Teaching and learning methods** | **Remarks** |
|---|---|---|
| 8.2.1. Identification of reversible covalent reactions. Exercises on identifying types of dynamic covalent bonds. | Problem-based seminar, group discussion, case studies | 1h/weak |
| 8.2.2. Mechanisms of dynamic covalent exchange. Mechanistic problems: acid-base catalysis, metathesis. | Problem-based seminar, group discussion, case studies | 1h/weak |
| 8.2.3. Reversible condensation reactions. Exercises on formation/hydrolysis of imines, hydrazones, oximes. | Problem-based seminar, group discussion, case studies | 1h/weak |
| 8.2.4. Disulfide bonds and boronic esters. Problems regarding S-S bond formation/exchange and boronic esters. | Problem-based seminar, group discussion, case studies | 1h/weak |

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| 8.2.5. Analysis of dynamic combinatorial libraries. Case studies: designing a DCL. | Problem-based seminar, group discussion, case studies | 1h/weak |
| 8.2.6. Templating and amplification in DCLs. Template-induced selectivity problems. | Problem-based seminar, group discussion, case studies | 1h/weak |
| 8.2.7. Macrocycle synthesis – case studies. Analysis of synthesis strategies: monomer-to-macrocycle vs. polymer-to-macrocycle. | Problem-based seminar, group discussion, case studies | 1h/weak |
| 8.2.8. Organic molecular cages – design and applications. Exercises on molecular cage design. | Problem-based seminar, group discussion, case studies | 1h/weak |
| 8.2.9. Orthogonal systems – design. Exercises on combining orthogonal DCC reactions | Problem-based seminar, group discussion, case studies | 1h/weak |
| 8.2.10. Self-sorting and molecular machines. Analysis of self-sorting examples. | Problem-based seminar, group discussion, case studies | 1h/weak |
| 8.2.11. Dynamic polymers – characterization and properties. Analysis of mechanical and self-healing properties. | Problem-based seminar, group discussion, case studies | 1h/weak |
| 8.2.12. Applications and perspectives – student presentations. Individual presentations and final discussion. | Problem-based seminar, group discussion, case studies | 1h/weak |

Bibliography:


1. Dynamic Covalent Chemistry: Principles, Reactions, and Applications, W. Zhang, Y. Jin, , John Wiley & Sons, Chichester, 2018.
2. From Supramolecular Chemistry Towards Constitutional Dynamic Chemistry and Adaptive Chemistry. J.-M. Lehn,* *Chem. Soc. Rev.* 2007, 36, 151–160.
3. Recent Progress in Polymers with Dynamic Covalent Bonds. H. Li, X. Zhang, *Macromol. Chem. Phys.* 2023, 224, 2300224.
4. Self-Healing and Shape-Shifting Polymers Controlled by Dynamic Covalent Chemistry. L. Zhao, *Macromol. Rapid Commun.* 2023, 44, 2300401.
5. Targeting Biomolecules with Reversible Covalent Chemistry. J. Li, *Acc. Chem. Res.* 2016, 49, 1144–1156.
6. Structural diversity ranging from oligonuclear complexes to 1-D and 2-D coordination polymers generated by tetrasubstituted adamantane and spirobifluorene derivatives. T. Mocanu, L. Pop, N.D. Hădade, S. Shova, L. Sorace, I. Grosu, M. Andruh, *Eur. J. Inorg. Chem.* **2019**, 5025–5038.
7. Examination of Structure-Activity Relationship of New *N*-Acylhydrazones A. G. Coman, A. Paun, C. C Popescu, N. D Hădade, A. Hanganu, A. M Mădălan, M. Matache *Rev. Roum. Chim.* **2020**, *65***,** 109-114.
8. Exploring Arylazo-3,5-Bis(trifluoromethyl)pyrazole Switches B. C. Enache, A. Hanganu, C. Tablet, C. C. Anghel, C. C. Popescu, A. Paun, N. D. Hădade, A. M. Mădălan, M. Matache *ACS Omega* **2022**, *7*, 39122–39135.
9. Planar Chiral p,p′-Terphenyl-Based Cyclophanes with Remarkable Enantiomer Stability: Synthesis, Theoretical Investigations, and Complexation Studies I. Stroia, M. E. Moisă, A. Pop, B. Legrand, A. Hanganu, N. D. Hădade,* Ion Grosu* *J. Org. Chem.* **2023**, *88*, 15647–15657.
10. Pillar [n] arenes– adaptive artificial water/ion/proton channels in membranes S. Daakour, N. D. Hădade, M. Barboiu *Tetrahedron Lett.*, **2024**, *145*, 155178.
11. Synthesis of dynamic N-acylhydrazone-based macrocycles N. Sandu, A. Hanganu, C. Popescu, A. M Demeter, A. G Mirea, A. Kuncser, C. Tăblet, N. D Hădade, M. Florea, D. P Funeriu, M. Matache, *J. Mat. Chem. A*, **2025**, *13,* 10232-10242.
12. Other articles from recent literature


**9. Evaluation**

| Type of activity | 9.1 Evaluation criteria[4] | 9.2 Evaluation methods[5] | 9.3 Percentage in the final grade |
|---|---|---|---|

[4] The evaluation criteria must directly reflect the learning outcomes targeted at the level of the degree programme respectively at the level of the subject. More specifically, the learning outcomes set out in the expected learning outcomes are assessed.

[5] Both final evaluation methods and ongoing evaluation strategies should be established.

| | | | |
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| 9.4. Course | Knowledge and understanding of fundamental concepts of dynamic covalent chemistry; capacity for synthesis, analysis and interpretation of DCvC reactions and systems. | Oral exam | 60 % |
| 9.5. Seminar/ laboratory | Active participation in discussions; quality of reports and presentations; capacity to apply knowledge to problem solving. | Continuous assessment (reports, presentations, participation) | 40% |
| | | | |
| 9.6 Minimum standard for passing | | | |
| Achieving a minimum grade of 5 (five), demonstrating knowledge of the basic concepts of dynamic covalent chemistry, the main types of reversible covalent reactions and fundamental applications. | | | |

**10. SDG labels (Sustainable Development Goals)[6]**

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | ○ | Sustainable Development Generic Label | | | | | | |
| 1 FĂRĂ SĂRĂCIE | 2 FOAMETE „ZERO" | 3 SĂNĂTATE ȘI BUNĂSTARE | 4 EDUCAȚIE DE CALITATE | 5 EGALITATE DE GEN | 6 APĂ CURATĂ ȘI SANITAȚIE | 7 ENERGIE CURATĂ ȘI LA PREȚURI ACCESIBILE | 8 MUNCĂ DECENTĂ ȘI CREȘTERE ECONOMICĂ | 9 INDUSTRIE, INOVAȚIE ȘI INFRASTRUCTURĂ |
| ○ | ○ | ○ | X | ○ | ○ | ○ | ○ | ○ |
| 10 INEGALITĂȚI REDUSE | 11 ORAȘE ȘI COMUNITĂȚI DURABILE | 12 CONSUM ȘI PRODUCȚIE RESPONSABILE | 13 ACȚIUNE CLIMATICĂ | 14 VIAȚA ACVATICĂ | 15 VIAȚA TERESTRĂ | 16 PACE, JUSTIȚIE ȘI INSTITUȚII EFICIENTE | 17 PARTENERIATE PENTRU REALIZAREA OBIECTIVELOR | No label applies |
| ○ | ○ | ○ | ○ | ○ | ○ | ○ | ○ | ○ |

Date of entry:
26.01.2026

Signature of course coordinator

Prof. dr. Niculina Daniela Hădade

Signature of seminar coordinator

Prof. dr. Niculina Daniela Hădade

Date of approval in CDSC:

Signature of the Director of the DSC

Prof. dr. Niculina Daniela Hădade

[6] Select a single label which, according to the *Implementation of SDG labels in the academic process*, best matches the subject. If the subject addresses sustainable development in a generic manner (i.e. by presenting/introducing the general framework of sustainable development, etc.), then the Sustainable Development generic label may be applied. If none of the labels describe the subject, select the last option: *"No label applies."*