



UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

SYLLABUS DEL CORSO

Organic Strategies for Materials Synthesis

2627-1-FSM02Q030-FSM02Q03001

Aims

Objectives

Organic conjugated materials are a relevant part of modern materials science. Aim of the course is to provide a detailed knowledge of the most common synthetic methods for the preparation of conjugated materials with electronic and optoelectronic application. Particular emphasis will be given to green chemistry compliant approaches

Knowledge and understanding

At the end of the course the student:

1. Understands the concept of conjugation in organic materials and correlates the extension of conjugation with optical, electrical and optoelectronic properties
2. Understands the features of the most common approaches for functionalization, arylation and olefination applied in the synthesis of organic materials
3. Can select the most appropriate synthetic approaches depending on the characteristics of the final material.

Applying Knowledge and understanding:

The student:

1. Knows the features of organic conjugated materials and understands the basic structure relationships that are relevant to devise suitable synthesis and functionalization strategies.
2. Knows the most relevant arylation strategies

3. Knows the most relevant olefination approaches.
4. Knows the state of the art approaches for the synthesis of conjugated polymers

Making judgments.

Given the structure of a conjugated molecule or polymer, the student is capable of devising a suitable synthetic approach for its preparation. Given a certain function that an organic molecule is required to perform, the student can propose functionalization strategies of molecules to optimize a certain feature.

Communication skills.

The student is trained in the reading, understanding and summarizing of scientific literature. Particular emphasis is given to the synthetic approaches and to the comparative evaluation of sustainability of various available approaches. The student possesses the specific terminology of the field, thus being in the position of discussing with counterparts possessing both a chemical and a materials science background. He possesses a "problem solving" attitude.

Learning skills.

The Student is able to extend what has been learned in classes to case studies not covered during the course. He is in particular able to autonomously manage the wide literature dedicated to the conjugated materials. He knows the research tools of the dedicated literature, including patents.

Contents

- Conjugation and aromaticity
- Features of organic conjugated materials
- Overview of synthetic methods for arylation and olefination reactions
- Metallorganic derivatives (ArLi and ArMgX) and their applications in synthesis
- Synthesis and functionalization of donor moieties
- Formylation and halogenation reactions
- Wittig & Horner-Hammonds reactions for the synthesis of conjugated linkages
- Pd mediated reactions
- Direct arylation reactions
- Synthesis of acceptor moieties
- Polymerizations
- Characterization techniques for conjugated polymers

Detailed program

- Conjugation and aromaticity
 - o Hybridization of C, N, O, P, S atoms
 - o Double and triple bonds
 - o Conjugated bonds
 - o Homo and heteroaromaticity
 - o Base knowledge on heterocyclic chemistry
- Features of organic conjugated materials

- o Structure of polyconjugated materials
- o Transport properties
- o Optical properties
- o Optoelectronic properties
- Overview of synthetic methods for arylation and olefination reactions
- Metallorganic derivatis (ArLi and ArMgX) and their applications in synthesis
- o Direct Litiation by deprotonation and halogen lithium exchange
- o Dance of halogen and regio stability of ArM
- o Grignard reagents preparation
- o Use of organic metal derivatives in synthesis
- Syntesis and functionalization of donor moieties
- o Halogenation and formilation (electrophilic halogenation reactions and Vilsmeier formilation, use of ArM)
- Reactions by Wittig and Horner-Hammonds for the synthesis of conjugated bridges
- Pd, Ni, Cu mediated reactions
- o Stille coupling
- o Suzuki coupling
- o Sonogashira coupling
- o Heck coupling
- o Buchwald-Hartwig coupling
- o Kumada coupling
- o Ullman coupling
- Direct arylation reactions
- Synthesis of acceptors
- o Condensation of Knoevenagel
- o Synthesis of polymethine dyes
- o Examples of synthesis and functionalization of heterocyclic acceptors
- Polymerizations
- Characterization techniques for conjugated polymers

Prerequisites

Chemistry of materials requires an interdisciplinary approach exploiting general and inorganic, organic, macromolecular and physical chemistry (thermodynamics and chemical equilibria).

An interdisciplinary foundation is thus required, including:

- General and Inorganic Chemistry.
- Organic Chemistry.
- Physical Chemistry (Thermodynamics and Chemical Equilibria)

Teaching form

The course is organized with in person lessons. Lectures will be also videotaped and made available on the e-

learning platform at the end of the course to support individual study.
Teaching language will be English.

Teaching strategy:

12 two-hour lectures, in person, Delivered Didactics

Textbook and teaching resource

•Books:

Synthetic Methods in Organic Electronic and Photonic Materials: A Practical Guide
Authors: Timothy Parker; Seth Marder
DOI: <https://doi.org/10.1039/9781839168833>
Paperback ISBN: 978-1-84973-986-3
EPUB ISBN: 978-1-78801-814-2
PDF ISBN: 978-1-83916-883-3
Special Collection: RSC eTextbook Collection
Publication date: 04 Aug 2015

The book is available in electronic e-book format on the library site at the following address:

https://search.ebscohost.com/login.aspx?direct=true&db=nlebk&AN=3579778&site=ehost-live&scope=site&ebv=EK&ppid=Page-__-1

Palladium reagents and catalysts. Author(s): Jiro Tsuji
First published: 23 April 2004
Print ISBN: 9780470850329 | Online ISBN: 9780470021200 | DOI: 10.1002/0470021209

•Annotated slides

•Video recording of classes (at the end of the course)

Semester

first semester.

Assessment method

The final mark for "Strategies for Materials Synthesis" is a composite score derived from the three modules (Organic, Inorganic, and Macromolecular).

- Overall Evaluation Criteria:

The assessment is conducted via oral examinations for each module. The final grade of Strategies for Materials Synthesis course is calculated as the average of the marks obtained in its three constituent modules: Inorganic Strategies for Materials Synthesis, Organic Strategies for Materials Synthesis and Macromolecular Strategies for Materials Synthesis

During the exam, the student will be required to answer 3–4 questions over a duration of approximately 20 minutes. One of these questions will be on a topic of the student's choice. The remaining questions will focus on the topics covered during the lectures with the aim to assess the ability to rearrange the concepts. Students will be encouraged to think about the possible use of their notions in practical examples/applications (problem solving).

Partial exams are not scheduled.

The evaluation criteria for the are as follows:

18-21: Sufficient Level

- Knowledge and Understanding: The student demonstrates a basic understanding of the concept of conjugation in organic materials and can identify the relationship between conjugation and the optical, electrical, and optoelectronic properties of materials. He recognize some common synthetic methods for preparing conjugated materials but may have gaps in their knowledge.
- Applying Knowledge and Understanding: The student can identify basic functionalization, arylation, and olefination strategies but may struggle to select the most appropriate synthetic approaches for specific materials.
- Making Judgments: The student shows limited ability to devise suitable synthetic approaches for given conjugated molecules or polymers and may have difficulty proposing functionalization strategies.
- Communication Skills: The student can read and summarize scientific literature but may lack clarity in discussing synthetic approaches and sustainability evaluations. Their use of specific terminology is basic.
- Learning Skills: The student demonstrates some ability to extend learned concepts to new case studies but relies heavily on course materials and shows limited engagement with the broader literature.

22-24: Good Level

- Knowledge and Understanding: The student has a good understanding of conjugation in organic materials and can explain how it affects material properties. He is familiar with several synthetic methods and can describe their features.
- Applying Knowledge and Understanding: The student can select appropriate synthetic approaches for specific materials and understands the most relevant arylation and olefination strategies.
- Making Judgments: The student can devise suitable synthetic approaches for specific conjugated molecules and propose functionalization strategies, although their solutions may lack depth or creativity.
- Communication Skills: The student effectively communicates their understanding of scientific literature, discussing synthetic approaches and sustainability with reasonable clarity. He use specific terminology appropriately but may still have room for improvement.
- Learning Skills: The student shows a good ability to manage the chemistry related to conjugated materials and can apply learned concepts to case studies, though he may still require guidance.

25-27: Very Good Level

- Knowledge and Understanding: The student demonstrates a strong understanding of conjugation and its implications for material properties. He can articulate the features of various synthetic methods and their applications in detail.
- Applying Knowledge and Understanding: The student effectively selects and justifies appropriate synthetic approaches for a range of materials, demonstrating a solid grasp of arylation and olefination strategies.
- Making Judgments: The student can autonomously devise suitable synthetic approaches for conjugated molecules and propose effective functionalization strategies, showing critical thinking in their judgments.

- **Communication Skills:** The student communicates their findings clearly and confidently, summarizing scientific literature and discussing sustainability evaluations with precision. He uses field-specific terminology effectively.
- **Learning Skills:** The student demonstrates strong independent learning skills and ability to apply knowledge to new case studies with minimal guidance.

28-30 with Honors: Excellent Level

- **Knowledge and Understanding:** The student exhibits an exceptional understanding of conjugation in organic materials and can correlate it with advanced optical, electrical, and optoelectronic properties. He possess comprehensive knowledge of synthetic methods and their implications for material design.
- **Applying Knowledge and Understanding:** The student expertly selects synthetic approaches for a wide variety of conjugated materials, demonstrating mastery of arylation and olefination strategies.
- **Making Judgments:** The student shows outstanding ability to devise suitable and efficient synthetic approaches for complex conjugated molecules and proposes functionalization strategies, demonstrating exceptional critical thinking and problem-solving skills.
- **Communication Skills:** The student excels in communicating complex ideas clearly and persuasively, effectively summarizing and critiquing scientific literature. He engage in discussions with peers from both chemistry and materials science backgrounds with confidence and authority.
- **Learning Skills:** The student demonstrates exceptional autonomy in learning and applying his knowledge to novel case studies.

Office hours

Upon request via e-mail

Sustainable Development Goals

AFFORDABLE AND CLEAN ENERGY
