

Materials design and selection for circular economy

Silvia Gross, Enrico Bernardo,
Laura Orian, Paolo Dolcet

Università degli Studi di Padova

In general, the course is aimed at providing the fundamentals of materials selection oriented to sustainability. In its interdisciplinary structure, the course is expected to lead to the following knowledge and skills:

Module 1: Materials in circular economy and eco-informed material choice (6 ECTS) – Gross, Bernardo

The main goal of this first module is to introduce eco-design and circularity-oriented design of materials for applications in different sectors. Specific goals are:

To understand materials in a circular economy dimension and their relevance in specific sectors.

To be able to identify, in the performance of a component, a series of "indices", or combinations of material properties to be optimised in order to reduce energy consumption and carbon footprint

To be able to recognise the several stages of materials life cycle and operate on them by means of "Eco-audits"

To be able to adjust materials selection according to the availability of raw materials.

Different classes of materials will be discussed and corresponding circular options discussed

Module 2: Design and selection of functional molecules and materials for sustainable synthesis and circularity (2 ECTS)- Orian

The main goal of the module is to illustrate how to design in silico a circular product and assess its physico-chemical properties. This approach requires the introduction of the fundamentals and applications of few topics of computational chemistry to predict and interpret structural and reactivity properties of functional molecules and materials.

1 ECTS devoted to computational laboratory activity and description of case-studies.

Module 3: Molecules and materials chemico-physical characterisation (1 ECTS) - Dolcet

This module aims at providing the students chemico-physical basis of selected analytical tools to characterise molecules and materials from the compositional, structural/morphological

(SEM, TEM) and functional point of view.

Course aims and topics: Gross

-  Materials Design and Selection_Gross_1 part_Introduction to the course.ppt
-  Materials Design and Selection_Gross_2 part_Resources and context.ppt
-  Materials Design and Selection_Gross_3 part_Raw materials materials features and classification.ppt
-  Materials Design and Selection_Gross_4 part_Ceramics and glasses.ppt
-  Materials Design and Selection_Gross_5 part_Composites.ppt
-  Materials Design and Selection_Gross_6 part_Concrete and cement.ppt
-  Materials Design and Selection_Gross_7 part_Nanomaterials.ppt
-  Materials Design and Selection_Gross_8 part_Circular Chemistry.ppt
-  Materials Design and Selection_Gross_9 part_Paper and textiles.ppt
-  Materials Design and Selection_Gross_10 part_The 9R and categorisation of EC.ppt
-  Materials Design and Selection_Gross_11_Circular options for materials classes_Construction.ppt
-  Materials Design and Selection_Gross_12_Circular options for materials classes_Glass.ppt
-  Materials Design and Selection_Gross_13_Circular options for materials classes_Ceramics refractories.ppt
-  Materials Design and Selection_Gross_14_Circular options for materials classes_Composites.ppt
-  Materials Design and Selection_Gross_15_Circular options for materials classes_Textiles.ppt
-  Materials Design and Selection_Gross_16_Substitution approaches.ppt

Assessment criteria:

The evaluation criteria consist of:

1. Completeness of the acquired knowledge
2. Property of technical terminology
3. Consistency and precision in the application of numerical algorithms and graphs
4. Comprehension of the multi-scale computational methodologies and of their application to the design in silico of a circular process and/or product.

Exam

The verification of the expected knowledge is carried out through a **written test**. The written exam consists of 12 questions (including some exercise), on the whole program of the course excluding the part of Prof. Orian (8 extra points assigned on the basis of classroom work). The sum of the scores determines the overall grade (maximum = 28 points, to which the points of Prof. Orian should be added). The maximum grade ("30/30 cum laude") is awarded for a final score of 33 points. 3 hours available.

Module 1: Materials in circular economy and eco-informed material choice

Gross, Bernardo

Introduction to materials: main features (composition, structure, morphology, structure-properties relationships), main classes (metals/alloys, polymers, ceramics/glasses) their relevance in main specific sectors (plastics, building & construction, metals, apparel & textiles, energy conversion and storage) in a circular economy perspective. Circular options for different classes of materials. Specific topics:

Basics on circular chemistry.

Embedding sustainability in the design/manufacturing of materials. Sankey diagrams of materials flow.

How to address criticality: material design to reduce CRM content and substitution approaches.

Introduction to material properties charts: development and use. Definition of materials indices: performance of a component according to a combination of properties; selection through charts and indices. Presentation of "pure" selection case studies, with discussion of the characteristic equations and derivation of selection indices. Materials selection with conflicting objectives: trade-off analysis.

Environmental impact monitoring methods. Case studies of graphical materials selection oriented to environmental sustainability (control of energy and carbon footprint) in primary production.

Materials life cycle: definition of boundaries, introductory remarks to LCA, principles of eco-auditing. Updates on environmental sustainability from inclusion of manufacturing step. Presentation and analysis of end-of-life options. Case studies of application of eco-audits: introduction to the CES (Cambridge Engineering Selector) software, comparison between disposable and reusable constructions, material substitution

Case studies on cost/environmental sustainability trade-off

Sustainability by means of material minimization: introduction of shape factors, with case studies.

Module 3: Molecules and materials chemico-physical characterisation (1 ECTS) – Dolcet

- The interaction between the electromagnetic radiation and matter is of paramount importance in order to characterize and gain insights on the chemico-physical properties of materials. Ultraviolet/Visible/Infrared (**UV/Vis/IR**) spectroscopies will be presented in terms of their basics, instrumentations and applications.
- Transfer of energy from/to a material of interest can be exploited to characterize a wide portfolio of materials. Basics on thermal gravimetry analysis (**TGA**), differential scanning calorimetry (**DSC**) etc. will be presented.
- Electron microscopy such as transmission electron microscopy (**TEM**) and scanning electron microscopy (**SEM**) will be shortly presented because they can provide morphological and compositional properties.
- Some case studies will be matter of this teaching.

Reference textbooks:

1. Principles of Instrumental Analysis, Seventh Edition 2016. Authors: D.A Skoog, F.J. Holler and S.R. Crouch.
2. Microstructural Characterization of Materials 2nd Edition 2008. Authors: D. Brandon and W.D. Kaplan.
3. Materials Science and Engineering AN INTRODUCTION, tenth edition 2018. Authors: W.D. Callister and D.G. Rethwisch.