UNIVERSITÀ DEGLI STUDI DI PALERMO

DEPARTMENT	Fisica e Chimica - Emilio Segrè
ACADEMIC YEAR	2021/2022
MASTER'S DEGREE (MSC)	CHEMISTRY
SUBJECT	ADVANCED INORGANIC CHEMISTRY
TYPE OF EDUCATIONAL ACTIVITY	B
AMBIT	50483-Discipline chimiche inorganiche e chimico-fisiche
CODE	01925
SCIENTIFIC SECTOR(S)	CHIM/03
HEAD PROFESSOR(S)	DUCA DARIO Professore Ordinario Univ. di PALERMO
OTHER PROFESSOR(S)	
CREDITS	8
INDIVIDUAL STUDY (Hrs)	136
COURSE ACTIVITY (Hrs)	64
PROPAEDEUTICAL SUBJECTS	
MUTUALIZATION	
YEAR	1
TERM (SEMESTER)	2° semester
ATTENDANCE	Mandatory
EVALUATION	Out of 30
TEACHER OFFICE HOURS	**DUCA DARIO** Monday 13:00 14:00 Studio del docente presso Ed.17. Tuesday 13:00 14:00 Studio del docente presso Ed.17. Wednesday 13:00 14:00 Studio del docente presso Ed.17. Thursday 13:00 14:00 Studio del docente presso Ed.17. Friday 13:00 14:00 Studio del docente presso Ed.17. Saturday 10:00 13:00 Studio del docente presso Ed.17.

DOCENTE: Prof. DARIO DUCA

PREREQUISITES	Inorganic-, organic- and physical-chemistry training of the first degree chemistry course. Quantum mechanics fundaments.
LEARNING OUTCOMES	- Ability to explain the chemical bond, the coordination capacity and the structural characteristics in terms of molecular but also of of solid-state models. - Ability to identify and use theoretical paradigms useful to explain the information deriving from different methods of characterization in the research field concerning materials related to the catalysis. - Ability to interpret the way in which topological, steric and electronic properties, influence the chemical properties of molecules or solid state fragments, in particular of the ones related to catalytic applications. - Ability to design and explain the electronic structure of materials used in catalysis and eventually in the renewable energy field. - Ability to apply knowledge on catalysis, using a unifying perspective able to reduce to one the different paradigms normally used to study the distinct aspects of seemingly unrelated catalytic systems: heterogeneous, homogeneous, enzymatic, etc. - Ability to learn, using technical books and scientific literature, topics related to the catalysis and chemistry of materials. - Communication skills on catalysis and on their conceptual bases and models.
ASSESSMENT METHODS	One written (4.5 credits) and one oral (3.5 credits) examen are planned. With the first i) the understanding of the concepts concerning either the point group or the translational symmetry and ii) the ability to use them in different chemical contexts are evaluated. With the second one, the learning of the course section, concerning catalysis as well as organometallic and cluster chemistry, in particular of those species used in catalysis, is examined. Positive exam scores, in both the examinations, are framed into five sets: excellent exams are assessed cum laude, distinguished ones with a mark in the range 30-27, good 26-23, more than sufficient 22-19 and just sufficient 18. The final grade will not be based on the weighted sum of both the exam components above.
EDUCATIONAL OBJECTIVES	The course is developed in a semester with classes. At first, in the course, the theory of groups and, more generally, the concept of symmetry, including translational symmetry, is taken up. In this first phase, very basic notions of graph theory are also introduced, useful for understanding concepts such as the aromaticity of inorganic systems and the consequent stability of given species of the elements of the main groups such as (boranes and their congeners) and metal clusters.. The organometallic chemistry with the cluster chemistry are deepened to start the second part of the course. These are presented as the basis for the development of the simplest mechanistic and synthetic schemas to be used in the study of catalysis. The latter is presented by introducing its historical bases, its principles – in the various application areas – and its modern and advanced tools, especially useful: i) to design eco-friendly and renewable synthetic routes of industrial processes and ii) to identify models that can be used to study the same industrial processes. Catalysis modeling is proposed as a bridge between the two parts of the course.
TEACHING METHODS	Lessons.
SUGGESTED BIBLIOGRAPHY	GROUP THEORY FOR CHEMISTS; George Davidson 1st Ed. — MACMILLAN EDUCATION Ltd. 1991. APPLICATIONS OF GRAPH THEORY AND TOPOLOGY IN INORGANIC CLUSTER AND COORDINATION CHEMISTRY; R. Bruce King —CRC Press Inc. 1992. CHIMICA INORGANICA; Gary L. Miessler, Donald A. Tarr — Piccin 2011. CATALYSIS Concepts and Green Applications; Gadi Rothenberg — WILEY-VCH Verlag GmbH & Co. 2008. CHEMICAL APPLICATIONS OF GROUP THEORY; F. Albert Cotton 3rd Ed. — John Wiley & Sons, Inc. 1991. CHIMICA INORGANICA DESCRITTIVA; Geoff Rayner-Canham, Tina Overton —EDISES 2017.

SYLLABUS

Hrs	Frontal teaching
2	Sketch on theorems and definitions of group theory
4	Molecular symmetry and symmetry groups
6	SALCs
22	Symmetry applications on molecular and solid state (inorganic) systems: orbital energy diagrams and band theory, electronic spectroscopy, vibrational spectroscopy (IR, Raman), orbital symmetry and chemical reactions (Woodward-Hoffmann paradigm), graph theory and topology: simple applications in inorganic chemistry
4	Crystallographic symmetry and crystalline solid state
6	Deepening on organometallic chemistry
2	Characterization of organometallic species and fragments

SYLLABUS

Hrs	Frontal teaching
4	Ligand reactivity in metal complexes
2	Homo- and hetero-atomic cluster-like compounds
12	Catalysis: from the models to the industrial applications