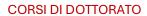UNIVERSITÀ DEGLI STUDI DI PADOVA

Course unit English denomination	**Advanced theoretical and mathematical methods to support and rationalise inorganic materials and molecular synthesis**
Teacher in charge (if defined)	GROSS Silvia, FRESH Barbara, ZERBETTO Mirco, MAZZI Anna, STOPPATO Anna, SALMASO Luigi
Teaching Hours	24
Number of ECTS credits allocated	3
Course period	06-09/2025
Course delivery method	☐ In presence ☐ Remotely ☒ Blended
Language of instruction	English
Mandatory attendance	☒ Yes (80 % minimum of presence) ☐ No
Course unit contents	The course aims at introducing modelling and statistical methods to support and rationalize materials synthesis. The course, with a strong interdisciplinarity, will encompass different sub-modules given by teachers of different discipline, ranging to inorganic chemistry, to computational chemistry, to statistics, to engineering. In particular, the course will provide a perspective of modern methods, based on multiscale classical and quantum approaches, for the characterization *in-silico* of synthetic inorganic processes, their implementation and engineering. Sub-modules: - introduction to a rational approach to inorganic synthesis (Silvia Gross, 4 h) - basics of thermodynamics supporting Life Cycle Assessment (Zerbetto 2 h) - introduction to Life Cycle Assessment (Stoppato, 3 h) - Life Cycle Assessment in Green Chemistry (Mazzi, 3 h) - introduction to on multiscale classical and quantum approaches, for characterization *in-silico* of synthetic inorganic processes (Zerbetto, Fresh 6 h) - introduction to DoE (assegnista Salmaso, 4 h) - examples (Gross, 2 h)
Learning goals	Knowledge: basics of mathematics, physics and Skills: understanding and applying the methods described in the lectures Competencies: Basics of multiscalde modelling of synthesis processes, DoE and LCA
Teaching methods	Frontal teaching
Course on transversal, interdisciplinary,	☒ Yes ☐ No

transdisciplinary skills	
Available for PhD students from other courses	☒ Yes ☐ No Students external to the PhD Course admitted upon evaluation of the CV by the teachers
Prerequisites (not mandatory)	Basics of mathematics, chemistry
Examination methods	The students will present a research project encompassing one or more of the approaches described in the lecture and will answer teachers questions.
Study material	Slides/articles provided by the teacher
Additional information (not mandatory)	max 3750 caratteri