Course: **Advanced theoretical and mathematical methods to support and rationalize materials and molecular synthesis**

Duration: 24 hours

Teacher(s): Silvia Gross, Antonino Polimeno, Anna Mazzi, Anna Stoppato, Gianluca Tondi, Luigi Salmaso

Curriculum: Scienze Chimiche

Description:

The course aims at introducing numerical, modelling and statistical methods to support and rationalise materials synthesis. The course, with a strong interdisciplinarity (chemistry, statistics, thermodynamics, modelling, forestal sciences) will encompass different sub-modules given by teachers of different discipline, ranging to inorganic chemistry, to computational chemistry, to statistics, to engineering.

- introduction to a rational approach to inorganic synthesis (Silvia Gross, 2 h)
- basics of thermodynamics supporting Life Cycle Assessment (Polimeno 3 h)
- introduction to LCA (Mazzi, Stoppato, 4 h)
- case studies on LCA supporting biomass valorisation for material synthesis (Tondi, 4 h)
- introduction to machine learning and modeling to design synthesis (Polimeno 6 h)
- introduction to DoE (Salmaso, 4 h)
- examples (Gross, 2 h)

Additional information: (*guest speakers, practical sessions, etc)*

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