



Minisimposio

“Statistical and LCA approaches to a rational synthesis of materials”

23 settembre 2022

ore 14.30-17:00

Aula G, Dipartimento di Scienze Chimiche

14.30-14.45

Introduction and motivation

Prof. Silvia Gross, Dipartimento di Scienze Chimiche, Università di Padova

14.45-15.30

Design of Experiments in the era of Artificial Intelligence

Prof. Luigi Salmaso, Dipartimento di Tecnica e Gestione dei Sistemi Industriali, Università di Padova

Abstract

Design of Experiments (DOE) is one of the main statistical techniques used in chemistry for variable screening and optimization. It is based on the simultaneous variation of multiple factors with the objective of finding the configuration of parameters that optimizes one or more responses of interest, e.g. reaction yield or product performance. Recently, DOE has been used as a method for collection of data that is then modelled through Machine Learning (ML) techniques. Main goals are usually to predict the response(s) at unobserved configurations of the inputs, or optimize the response(s) while at the same time minimizing the number of experimental trials. In this talk the advantages and possible applications of the DOE+ML methodology in the field of materials chemistry are discussed.

15.30-16.20

Life Cycle Assessment and its possible application in the field of materials chemistry.

Prof. Anna Mazzi, Prof. Anna Stoppato, Dipartimento di Ingegneria Industriale, Università di Padova

Abstract

Life Cycle Assessment (LCA) is a standardized methodology to evaluate the environmental burdens associated with a product or service through the entire life cycle (“from cradle to grave”) by identifying and quantifying energy and materials used, and emissions and wastes released to the environment (input-output analysis) and assessing the impacts on the ecosystem (impact assessment evaluation). The entire life cycle of the product, process, or activity is included in the analysis, encompassing extracting and processing raw materials, manufacturing, transportation and distribution, use, reuse, maintenance, recycling, and final disposal. Covered by international standards, LCA studies can support researchers and companies to understand the environmental profile of products, identify preferable options, improve the environmental performance, and compare alternative scenarios. In this talk the main concepts and possible applications of LCA in the field of materials chemistry are discussed.

16.20-17.00

Coffee break and discussion

Prof.ssa Silvia Gross

Il Direttore del Dipartimento
Prof. Michele Maggini