Course: **Notions of machine learning for chemistry**

Duration: 24 hours

Teacher(s): **Antonino Polimeno**

Curriculum: Professor of Physical Chemistry at DISC UniPD - Research activities are mainly dedicated to the interpretation of physico-chemical observables and chemical reactivity in non-ordered media, with an emphasis on soft materials and biological substrates. Current main interests lie in the development of models for interpreting spectroscopic signatures of structural and dynamic properties (e.g. magnetic resonance and optical spectroscopic data) in complex molecular systems (e.g. membranes, nanoaggregates, proteins). Main theoretical methods employed are based on projection operators and/or resummation techniques, many-body Fokker-Planck operators coupled with variational treatments.

http://www.chimica.unipd.it/antonino.polimeno

http://www.chimica.unipd.it/theochem

Description: - Chemistry and data (2h A)

- Computational learning (4h A + 2h E)

- Artificial neural networks (4h A + 2h E)

- Genetic algorithms (2h + 1h E)

- Machine learning for chemistry (6h + 1h E)

Additional information: hands on demonstrations and exercises will be carried on at the computational facilities of DiSC