

## Appunti di Fisica '23

**30 marzo, ore 15:00**

Sala Seminari, CNR-IPCF

### Machine learning methods in computational materials science (and beyond)

**A. Marco Saitta**

(IMPMC, Sorbonne Université/CNRS/Muséum National d'Histoire Naturelle - Paris France)

In recent years, machine learning has transformed scientific research, through the combination of the maturity of numerous approaches and algorithms, and the exponential growth of computing power. These approaches have already a dramatic impact in computational materials science, and will very likely have enormous impacts also in experimental characterization of matter and materials: from spectroscopy to imaging, a whole range of methods based on the exploitation of large databases has appeared. During this seminar, I will introduce the basic principles of machine learning, which are essential for the proper definition, optimization, validation, and use of a model. In a second part, I will present some examples of machine learning approaches in atomistic simulations, and, if time allows, in experimental characterization in materials science.

<https://appuntidifisicamessina.wordpress.com>