



# Seminar@ISM

organized by  
Communications Group



**CNR**  
Istituto di Struttura  
della Materia

## When?

April 16, 2025  
10:00 AM (CEST)

## Where?

@ Aula IB09  
Area di Ricerca -  
CNR Tor Vergata  
Rome



**Energy & Environment**

# 16

April 2025

## Gabriele Saleh

Istituto Italiano di Tecnologia  
Italy

### ***Big data and machine learning in materials science: toward data- driven semiconductor design***

*Data science and artificial intelligence are revolutionizing our world, and materials science is no exception. In the past, the ability to perform extensive quantum chemical simulations has accelerated the pace of materials design. In the near future, we may overcome the need for resource-intensive computations by leveraging existing data. By combining data mining with intelligently crafted machine learning (ML) algorithms, we can design new materials with tailored properties more efficiently than ever before.*

*This talk will explore data-driven approaches to designing and investigating materials. It will be structured in two parts: first, a general overview of big data and machine learning techniques in materials science; and second, a showcase of our platform for semiconductor materials discovery.*

*The first part will start with a pedagogical introduction on the general concept of ML. This will be followed by a discussion on materials databases and on the main applications of ML in materials science.*

*The second part of the talk will focus on the computational platform for data-driven semiconductors design developed by our group. Our platform: i) integrates the major materials databases into a unified interface, and ii) leverages various ML methods to predict material properties based on chemical composition. While containing features tailored for semiconductors, the platform is adaptable to any type of material. It aims to accelerate materials discovery through efficient screening.*

**Info at**

**[www.ism.cnr.it/seminar-ism](http://www.ism.cnr.it/seminar-ism)**

**[aldo.dicarlo@ism.cnr.it](mailto:aldo.dicarlo@ism.cnr.it)**

