



# Seminar@ISM

organized by  
Communications Group



**CNR**  
Istituto di Struttura  
della Materia

## When?

March 13, 2025  
3:30 PM (CET)

## Where?

@ Aula IB09  
Area di Ricerca -  
CNR Tor Vergata  
Rome



**Energy & Environment**

# 13

March 2025

## Ute Kaiser

Ulm University  
Germany

### ***Properties of Electron-Beam Functionalized Two-Dimensional Inorganic and Organic Materials and Heterostructures***

*A detailed understanding of electron-beam interactions with materials is essential for utilizing the unique chromatic- and spherical-aberration-corrected low-voltage SALVE instrument to both image and functionalize two-dimensional (2D) inorganic materials and heterostructures at the atomic scale.*

*In this talk, we combine density functional theory-based molecular dynamics simulations with U-Net-based fully convolutional neural network (FCN) analysis to understand the emergence of new phases and functionalities in various 2D inorganic materials, including transition metal dichalcogenides (TMDs), transition metal phosphorus trichalcogenides (TMPTs), and heterostructures composed of 2D perovskites and 2D crystalline lithium.*

*In the final part of the talk, we demonstrate that, under certain conditions, the low-voltage TEM approach can also be applied to image 2D organic materials at the near atomic scale.*

**Info at**

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

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**Ute Kaiser**

