Department of Chemistry, Biology
and Biotechnology of the
University of Perugia

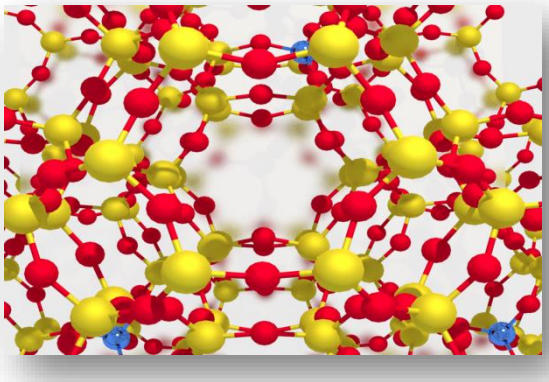
A.D. 1308
unipg
DIPARTIMENTO DI CHIMICA,
BIOLOGIA E BIOTECNOLOGIE
DIPARTIMENTO DI ECCELLENZA

# SEMINAR NOTICE

## On Wednesday 26th October 2022

## at 15:30 in room A

## of the Department of Chemistry, Biology and Biotechnology



**Dr. Federico Brivio**
*Weizmann Institute of Science*
*e-mail:* federico.brivio@weizmann.ac.il

**will give the seminar:**

## *"Two different declinations of DFT: thermodynamics and NMR"*

*Density functional theory (*DFT) permeates several fields of research in nowadays chemistry.
In this talk, we present two recent examples of DFT calculations used in conjunction with other analysis methods.
The first covers the **pairing of DFT results and statistical thermodynamics** to predict the properties of hybrid perovskites alloys.
Hybrid perovskites have experienced a boom of interest in the last decade because of their incredible efficiency if employed as photovoltaic materials. However, they present some limitations due to their chemical stability. To pinpoint this problem, we employed the generalized *quasi-chemical approximation* (GQCA) to rationalize the degradation mechanisms present in the material.
The second example regards ***solid-state NMR* (ssNMR) of zeolites.** $^{27}$Al ssNMR is the technique of choice for the characterization of Al environments in zeolite, but it is experimentally challenging due to the presence of quadrupolar effects, and lack of control on the *in-operando* conditions of the measure. To support the interpretation of experimental data, we employed **machine learning analysis of the DFT dataset** to highlight the critical structural-descriptors of zeolite structures and investigate and understand how experimental conditions reflect upon them.

All those interested are invited to participate.

Prof. Filippo De Angelis