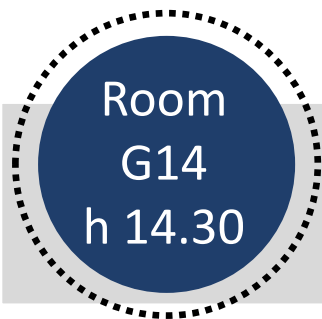


# The Chemist's Interactions

Seminars @ the Chemistry Department



Friday, 23<sup>rd</sup> May 2025

## Cristiana Di Valentin

Dipartimento di Scienza dei Materiali  
University of Milan-Bicocca



### Architecting Graphene Interfaces and Functionalized Nanoparticles for Nanotechnology and Bionanoscience

Interesting structural and electronic effects are observed when electronically or chemically doped graphene is interfaced with metal/metal oxide surfaces. In the first part of this talk we review some examples that have been simulated in our group by means of density functional theory (DFT) calculations and compared with experimental results: N- or Co-doped graphene interfaced with Ni(111), Fe-doped graphene interfaced with Pt(111) or graphene interfaced with Al<sub>2</sub>O<sub>3</sub>(0001).

The second part of the talk is devoted to functionalized transition metal oxide nanoparticles (i.e. TiO<sub>2</sub> and Fe<sub>3</sub>O<sub>4</sub>) for biomedical applications. Atomic models of realistic size (2-4 nm, i.e. 800-4000 atoms) are used to simulate, at a quantum mechanical level of theory in combination with classical molecular dynamics, the structural, electronic and magnetic properties of these nanosystems, their interaction with light and with the aqueous environment. Surface functionalization with stabilizing polymers or functionalizing molecular species for drug delivery, targeting and imaging is also discussed.

**Selected references:** *Carbon* 171 (2021) 704; *J Phys Chem Lett* 11 (2020) 8887; *Carbon* 176 (2021) 253; *Carbon* 201 (2023) 881; *Nat Catal* 4 (2021) 850; *Sci Adv* 10 (2024) eado8956; *Ang Chem Int Ed* (2025) e202421757; *Nanoscale* 15 (2023) 7909; *Nanoscale* 14 (2022) 12099; *JCIS* 627 (2022) 126; *Nanoscale* 14 (2022) 5121; *Nanoscale* 16 (2024) 4063; *Npj Comp Mater* 11 (2025) 20; *JCR* 379 (2025) 344



The event will be streamed on  
MS Teams for external participants!

For registrations: [seminari.dipchi@unimi.it](mailto:seminari.dipchi@unimi.it)



UNIVERSITÀ  
DEGLI STUDI  
DI MILANO