

CENIDE & WIN Seminar Series on 2D-MATURE

DFG IRTG 2803 & NSERC CREATE



Cristiana Di Valentin

Università di Milano Bicocca

“Interfacing doped graphene with metal/metal oxide surfaces or molecular layers”

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10:00 a.m. ET / 16:00 p.m. CET

Cristiana Di Valentin graduated in Chemistry in 1997 at the University of Pavia where she received her Ph.D. degree in Chemical Sciences in 2000 in collaboration with the Technische Universität München. She also holds a Master's degree in Materials Science. She was appointed by the University of Milano-Bicocca as Assistant Professor in 2002, as Associate Professor in 2012, and as Full Professor of General and Inorganic Chemistry in 2018. She has been a postdoc or a visiting scientist at Princeton University, Technische Universität München, Universitat de Barcelona, and Ecole Nationale Supérieure de Paris. Her research activity spans from *ab initio* computational studies of semiconducting oxides and bidimensional materials for catalysis, energy and sensing applications to multiscale modeling of bioinorganic hybrid nanosystems for biomedical applications. Professor Di Valentin has coauthored about 230 publications in peer-reviewed journals. She was awarded with an ERC Consolidator Grant (2016–2022) entitled: Smart bioinorganic hybrids for nanomedicine.

Interesting structural and electronic effects are observed when electronically or chemically doped graphene is interfaced with metal/metal oxide surfaces or molecular layers. In 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), B-doped graphene interfaced with Ir(111) and Ni(111) or graphene interfaced with Al₂O₃(0001); p-type doped graphene interfaced with a nickel-phthalocyanine (NiPc) monolayer or functionalized with tetrazine.

References

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