Curriculum Vitae

# Aldo Ugolotti


Contacts

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2023 – current occupation

## Fixed-time Research fellow (RTDA)

- Theoretical-computational research activity: first-principles investigation of the structure and of the electronic, elastic and thermodynamic properties of bulk and surfaces of semiconductors with application in the field of power electronics. Understanding of the epitaxial growth through models based on the classical nucleation theory, including parameters calculated by quantum-mechanical simulations based on the density functional theory (DFT) or by solving mechanical model through finite element methods (FEM).
- Research carried out within the group of Prof. L. Miglio, with collaboration with international groups, with focus on polymorph phases of large-bandgap semiconductor oxides, and Al- or Si-based oxides as substrate.
- Funding from grant PNRR 2022 Centro Nazionale Mobilità Sostenibile Missione 4.2.1.4 (MOST).

2019 – 2023

## Post-doc researcher c/o Università di Milano-Bicocca

- Theoretical-computational research activity: first-principles investigation of the structure, the electronic ground and excited state properties and the reactivity of systems of interest for chemical applications. Analysis of trends and comparison with experimental results, such as tunneling electron microscopy/spectroscopy STM/STS, resonant/non-resonant photo-excitation of core electrons XPS/NEXAFS/UPS, infrared and optical spectroscopies.
- Research carried out within Prof. C. Di Valentin's group, in collaboration with external experimental groups, with focus on both semiconductor or metallic surfaces, two-dimensional, graphene-like materials, both supported and free-standing, including the role of geometrical defects and doping/functionalization through organic molecules or single atoms.
- Funding from grant PRIN n. 2017NYPHN8 (Metal Activated 2D cArbon-based platforMs, MADAM).

## TEACHING ACTIVITY

Supervising theses

Tutoring and supervising the thesis work of Mater and Ph. D. students.

Teaching activity

### Elements of Experimental Methods

- First-year class, in the Bachelor degree in Materials Science and Nanotechnology, Università degli Studi di Milano-Bicocca
- Supervising and tutoring the students during the practical activities in the laboratory.
- AY 2024-2025
- AY 2023-2024

## EDUCATION

2016 - 2019

### Ph. D. in Materials Science and Nanotechnology

Università degli Studi di Milano-Bicocca

- Thesis title "Investigating metal-organic/inorganic interfaces with different dimensionalities from first-principles" , carried out at the Department of Materials Science, supervisor Prof. Gian Paolo Brivio, co-supervisor: Dott. Guido Fratesi.
- Theoretical-computational research activity: first-principles investigation of the structure, the electronic ground and excited state properties of systems with application in the field of opto-electronics.
- Focus on metallic surfaces and their interfaces with organic and inorganic molecules, of two-dimensional materials, such as graphene or silicene.
- Visiting Ph. D. student experience at the University of Central Florida (Orlando, US) in the group of Prof. A. Kara

2012 - 2016 **Master Degree in Physics**

Università degli Studi di Milano-Bicocca

- Curriculum of Condensed Matter Physics, thesis title "*Ab initio* investigation of the adsorption of aromatic molecules on a platinum surface" carried out at Department of Materials Science. Supervisor: Prof. Gian Paolo Brivio, co-supervisor: Dott. Guido Fratesi, grade 110/110 cum laude.

2003 - 2012 **Bachelor degree in Physics**

Università degli Studi di Milano, via Celoria, Milano

- Curriculum of General Physics thesis title "Studio di stelle di neutroni isolate in banda X, tramite i dati del satellite XMM-Newton", carried out at INAF-IASF CNR Milano. Internal supervisor Prof. Pierre Pizzochero, external supervisor, Dott. Andrea Tiengo.

## SCIENTIFIC CONTRIBUTION

### Publications

1. *"Interface energies of $Ga_2O_3$ phases with the sapphire substrate and the phase-locked epitaxy of metastable structures explained"*
   Bertoni I., Ugolotti A., Scalise E., Bergamaschini R., Miglio L.
   J. Mat. Chem. C 13, 1469, 2025
2. *"Surface and volume energies of α-, β-, and κ-$Ga_2O_3$ under epitaxial strain induced by a sapphire substrate"*
   Bertoni I., Ugolotti A., Scalise E., Miglio L.
   J. Mat. Chem. C 12, 1820, 2024
3. *"CO Adsorption on a Single-Atom Catalyst Stably Embedded in Graphene"*
   Perilli D., Chesnyak V., Ugolotti A., Panighel M., Vigneri S., Armillotta F., Naderasli P., Stredansky M., Schied M., Lacovig P., Lizzit S., Cepek C., Comelli G., Brune H., Africh C., Di Valentin C.
   Angewandte Chemie – Int. Ed. 64, 2025
4. *"Light-Induced Transformation of Virus-Like Particles on $TiO_2$"*
   Kohantorabi M., Ugolotti A., Sochor B., Roessler J., Wagstaffe M., Meinhardt A., Beck E., Dolling D., Garcia M., Creutzburg M., Keller T., Schwartzkopf M., Vayalil S., Thuenauer R., Guédez G., Löw C., Ebert G., Protzer U., Hammerschmidt W., Zeidler R., Roth S., Di Valentin C., Stierle A., Noei H.
   ACS Applied Materials & Interfaces 16, 37275, 2024
5. *"Insights into the active nickel centers embedded in graphitic carbon nitride for the oxygen evolution reaction"*
   Rossetti N., Ugolotti A., Cometto C., Celorrio V., Drazic G., Di Valentin C., Calvillo, L.
   J. Mat. Chem. A 12, 6652, 2024
6. *"Scalable bottom-up synthesis of Co-Ni-doped graphene"*
   Chesnyak V., Perilli D., Panighel M., Namar A., Markevich A., Bui T., Ugolotti A., Farooq A., Stredansky M., Kofler C., Cepek C., Comelli G., Kotakoski J., Di Valentin C., Africh C.
   Science Advances 10, 1, 2024
7. "*Vitamin C Affinity to $TiO_2$ Nanotubes: A Computational Study by Hybrid Density Functional Theory Calculations*"
   Ugolotti A., Dolce M., Di Valentin C.
   Nanomaterials 14, 261, 2024
8. "*Adsorption and Inactivation of SARS-CoV-2 on the surface of anatase $TiO_2$(101)*"
   Kohantorabi M., Wagstaffe M., Creutzburg M., Ugolotti A., Kulkarni S., Jeromin A., Krekeler T., Feuerherd M., Herrmann A., Ebert G., Protzer U., Guéde G., Löw C., Thuenauer R., Schlueter C., Gloskovskii A., Keller T., Di Valentin C., Stierle A., Noei H.
   ACS Applied Materials and Interfaces 15, 8770, 2023
9. *"In-Plane Hydrogen Bonds and Out-of-Plane Dipolar Interactions in Self-Assembled Melem Networks"*
   Ugolotti A., Lanzilotto V., Grazioli C., Schio L., Zamalloa-Serrano J., Stredansky M., Zhang T., de Simone M., Ferraro L., Floreano L., Coreno M., Puglia C., Di Valentin C.
   J. Phys. Chem. C 127, 11307, 2023
10. "*Trends in excitonic, vibrational and polaronic properties of graphitic carbon nitride polymorphs*"
    Ugolotti A. e Di Valentin C.
    Applied Surface Science 608, 155164, 2023
11. "*Ab-Initio Spectroscopic Characterization of Melem-Based Graphitic Carbon Nitride Polymorphs*"
    Ugolotti A. e Di Valentin C.
    Nanomaterials 11, 1863, 2021
12. "*Copper single-atoms embedded in 2D graphitic carbon nitride for the $CO_2$ reduction*"
    Cometto C., Ugolotti A., Grazietti E., Moretto A., Bottaro G., Di Valentin C., Calvillo L., Granozzi G.

npj 2D Materials and Applications 5,63, 2021

13. "*Inside-out growth method for high-quality nitrogen-doped graphene*"
    Fiori S., Perilli D., Panighel M., Cepek C., Ugolotti A., Sala A., Liu H., Comelli G., Di Valentin C., Africh C.,
    Carbon 171, 704, 2021
14. "*Nontrivial central-atom dependence in the adsorption of M-TPP molecules (M=Co, Ni, Zn) on Fe(001)-p(1×1)O*"
    FratesiG., Achilli S., Ugolotti A., Lodesani A., Picone A., Brambilla A., Floreano L., Calloni A., Bussetti G.
    Applied Surface Science 530, 147085, 2020
15. "*Coverage-dependent electronic and optical properties of H- and F-passivated Si/Ag(111) from first principles*"
    Ugolotti A., Brivio G. P., Fratesi, G.
    Phys. Rev. B 101, 195413, 2020
16. "*Fingerprints of $sp^1$ hybridized C in the near-edge X-ray absorption spectra of surface grown materials*"
    Fratesi G. , Achilli S., Manini N., Onida G., Baby A., Ravikumar A., Ugolotti A., Brivio G. P., Milani A., Casari C. S.
    Materials 11, 2556, 2018
17. "*Chemisorption of pentacene on Pt(111) with little molecular distortion*"
    Ugolotti A., Harivyasi S. S., Baby A., Dominguez M., Pinardi A. L., López M. F., Martín-Gago J. A., Fratesi G., Floreano L., Brivio G. P.
    J. Phys. Chem. C 121, 22797, 2017

## Conferences and workshops

1. Talk "*Interpretation of the competition between k and b phases with supersaturation in MOVPE growth of $Ga_2O_3$ on c-oriented sapphire*", ICG Conference, Lecce, 2025
2. Invited talk "*Characterization of SARS-CoV-2 adsorption on $TiO_2$ through ab-initio core-level spectroscopy*", CORAERO summer school, sincrotrone Desy, Amburgo (DE), 2024
3. Poster "First-principle approach to $Ga_2O_3$/Si and $Ga_2O_3$/3C-SiC interfaces", IWGO GraFOx, Berlin (DE), 2024
4. Invited talk "*Structural, electronic and spectroscopic properties of graphitic carbon nitride: interplay between theory and experiments*", workshop "From surfaces to devices: novel perspectives from nanostructured oxides and carbon materials", Università Cattolica del Sacro Cuore, Brescia, 2022
5. Talk "*Theoretical characterization of graphitic carbon nitride polymorphs: insights into the structural, electronic and spectroscopic properties*", 35th ECOSS, Luxembourg, 2022
6. Talk "*Graphitic carbon nitride allotropes: theoretical characterization of pristine, H-, O-, $NH_2$- and Cu-functionalised structures*", EMRS Spring Meeting, virtuale, 2021
7. Talk "*Electronic and optical properties of hydrogentated Silicene on Ag(111): a computational study*", Materials.it, Bologna, 2018
8. Poster "*Hydrogenated Silicene on Ag(111): a theoretical investigation through optical excitations*", 23° ETSF workshop on electronic excitations, Milano, 2018
9. Talk "*Tuning the electronic properties of Silicene through half-hydrogenation or Graphene support*", 6° meeting internazionale sul Silicene (IMS), Soleil Orsay (FR), 2017
10. Talk "*Chemisorption of Pentacene on Pt(111) with little molecular distortion*", Fismat, Trieste, 2017