Dr Daniele Perilli (CV is updated as 06/02/2025)

Junior Assistant Professor (RTDa)
CHEM-03/A – General and Inorganic Chemistry

University of Milano-Bicocca, Department of Materials Science
via R. Cozzi 55, 20125 Milano (MI), Italy

email: daniele.perilli@unimib.it

RESEARCH INTEREST

D. Perilli's scientific interests are related to the design and development of models and calculations using first-principles methods for the structural, electronic, and chemical reactivity description of the following systems:

1. 2D materials (e.g., graphene, hexagonal boron nitride, tungsten diselenide) functionalized with defects, dopants, or molecules for gas sensing applications, including medical sensing.
2. Interfaces between 2D materials and metal surfaces for catalysis and electrocatalysis.
3. Single metal atoms supported in 2D matrices or on surfaces for catalysis and electrocatalysis.
4. Electrocatalysts in chemical processes underlying devices for energy or hydrogen production, such as fuel cells or water-splitting cells.

CAREER

Apr 2023 – today	**Fixed-Time Assistant Professor** (RTD-a), University of Milano-Bicocca, Milano, Italy.
Nov 2020 – Apr 2023	**Post-Doc**, University of Milano-Bicocca, Milano, Italy.
Oct 2019 – Mar 2020	**Visiting PhD**, Karlsruhe Institute of Technology, Karlsruhe, Germany.
Apr 2017 – Sep 2017	**Research fellowship**, University of Milano-Bicocca, Milano, Italy.

EDUCATION

Dec 2020 – Apr 2021	**24 CFU for teaching (FIT)**, University of Milano-Bicocca, Milano, Italy.
Nov 2017 – Feb 2021	**PhD Materials Science**, University of Milano-Bicocca, Milano, Italy. Rank: cum laude.

Oct 2014 – Feb 2017 **MSc Chemical Sciences and Technologies**, University of Milano-Bicocca, Milano, Italy. Marks: 110/110 cum laude.

Oct 2011 – Oct 2014 **BSc Chemical Sciences and Technologies**, University of Milano-Bicocca, Milano, Italy. Marks: 110/110 cum laude.

AWARDS

2023 "**Premio Giovani Talenti**", Young Talents Award of the University of Milano-Bicocca (Italy) with the sponsorship of the Accademia Nazionale dei Lincei (Italy) – 2023 Edition. Motivation: "For his work on modeling the behavior of graphene-based hybrid nanostructures". Winner of the Third Prize.

PUBLICATIONS LIST

1 – G. Fazio, L. Ferrighi, **D. Perilli**, C. Di Valentin, "*Computational electrochemistry of doped graphene as electrocatalytic material in fuel cells*", **International Journal of Quantum Chemistry**, 2016, 116 (22), 1623-1640.

2 – C. Ronchi, M. Datteo, **D. Perilli**, L. Ferrighi, G. Fazio, D. Selli, C. Di Valentin, π "*Magnetism of Carbon Monovacancy in Graphene by Hybrid Density Functional Calculations*", **The Journal of Physical Chemistry C**, 2017, 121 (15), 8653-8661. (***Co-First Author***)

3 – L. Ferrighi, **D. Perilli**, D. Selli, C. Di Valentin, "*Water at the Interface Between Defective Graphene and Cu or Pt (111) Surfaces*", **ACS Applied Materials and Interfaces**, 2017, 9 (35), 29932-29941.

4 – **D. Perilli**, D. Selli, H. Liu, E. Bianchetti, C. Di Valentin, "*h-BN Defective Layers as Giant N-Donor Macrocycles for Cu Adatom Trapping from the Underlying Metal Substrate*", **The Journal of Physical Chemistry C**, 2018, 122 (41), 23610-23622. (***First Author***)

5 – T.H. Nguyen, **D. Perilli**, M. Cattelan, H. Liu, F. Sedona, N. A. Fox, C. Di Valentin, S. Agnoli, "*Microscopic insight into the single step growth of in-plane heterostructures between graphene and hexagonal boron nitride*", **Nano Research**, 2019, 12 (3), 675-682.

6 – **D. Perilli**, D. Selli, H. Liu, C. Di Valentin, "*Computational Electrochemistry of Water Oxidation on Metal-Doped and Metal-Supported Defective h-BN*", **ChemSusChem**, 2019, 12, 1995-2007. (***First Author***)

7 – H. Liu, **D. Perilli**, M. Dolce, C. Di Valentin, "*Insight into the Na adsorption on* $WSe_{2x}S_{2(1-x)}$ *monolayers: a hybrid functional investigation*", **Journal of Physics: Condensed Matter**, 2020, 32, 395001.

8 – S. Fiori, **D. Perilli**, M. Panighel, C. Cepek, A. Ugolotti, A, Sala, H. Liu, G. Comelli, C. Di Valentin, C. Africh, "*'Inside out' Growth Method for High-Quality Nitrogen-Doped Graphene*", **Carbon**, 2021, 171, 704-710.

9 – **D. Perilli**, S. Fiori, M. Panighel, H. Liu, C. Cepek, M. Peressi, G. Comelli, C. Africh, C. Di Valentin, "*Mechanism of CO Intercalation Through the graphene/Ni(111) interface and Effect of Doping*", **The Journal of Physical Chemistry Letters**, 2020, 11 (20), 8887-8892.

10 – S. Del Puppo, V. Carnevali, **D. Perilli**, F. Zarabara, A. Lodi Rizzini, G. Fornasier, E. Zupanič, S. Fiori, L.L. Patera, M. Panighel, S. Bhardwaj, Z. Zou, G. Comelli, C. Africh, C. Cepek, C. Di Valentin, M. Peressi, "*Tuning graphene doping by carbon monoxide intercalation at the Ni(111) interface*", **Carbon**, 2021, 176, 253-261.

11 – **D. Perilli**, C. Di Valentin, F. Studt, "*Can Single Metal Atoms Trapped in Defective h-BN/Cu(111) Improve Electrocatalysis of the H_2 Evolution Reaction?*", **The Journal of Physical Chemistry C**, 2020, 124 (43), 23690–23698.

12 – T. Kosmala, A. Baby, M. Lunardon, **D. Perilli**, H. Liu, C. Durante, C. Di Valentin, S. Agnoli, G. Granozzi, "*Operando visualization of the hydrogen evolution reaction with atomic-scale precision at different metal–graphene interfaces*", **Nature Catalysis**, 2021, 4 (10), 850-859.

13 – **D. Perilli**, R. Breglia, C. Di Valentin, "*Using Coordination Chemistry Concepts to Unravel Electronic Properties of SACs in Bidimensional Materials*", **The Journal of Physical Chemistry C**, 2022, 126 (23), 9615–9622.

14 – S. Freddi, **D. Perilli**, L. Vaghi, M. Monti, A. Papagni, C. Di Valentin, L. Sangaletti, "*Pushing Down the Limit of NH_3 Detection of Graphene-Based Chemiresistive Sensors through Functionalization by Thermally Activated Tetrazoles Dimerization*", **ACS Nano**, 2022, 16 (7), 10456-10469.

15 – A. Casotto, G. Drera, **D. Perilli**, S. Freddi, S. Pagliara, M. Zanotti, L. Schio, A. Verdini, L. Floreano, Cr. Di Valentin, L. Sangaletti, "*π-Orbital mediated charge transfer channels in a monolayer Gr–NiPc heterointerface unveiled by soft X-ray electron spectroscopies and DFT calculations*", **Nanoscale**, 2022, 14 (36), 13166-13177.

16 – M. Stojkovska, **D. Perilli**, J. E. Barcelon, M. Smerieri, G. Carraro, T. H. Dinh, L. Vattuone, M. Rocca, G. Bracco, M. Dell'Angela, R. Costantini, A. Cossaro, L. Vaghi, A. Papagni, C. Di Valentin, L. Savio, "*Well-ordered surface metal atoms complexation by deposition of Pd cyclometallated compounds on Ag (110)",* **Applied Surface Science**, 2022, 606, 154960. (***Co-First Author***)

17 – M. G. Cuxart, **D. Perilli**, S. Tömekce, J. Deyerling, F. Haag, M. Muntwiler, F. Allegretti, C. Di Valentin, W. Auwärter, "*Spatial Segregation of Substitutional B Atoms in Graphene Patterned by the Moiré Superlattice on Ir(111)*", **Carbon**, 2023, 201, 881-890.

18 – J. E. Barcelon, M. Stojkovska, **D. Perilli**, G. Carraro, M. Smerieri, L. Vattuone, M. Rocca, G. Bracco, M. Dell'Angela, R. Costantini, A. Cossaro, L. Vaghi, A. Papagni, C. Di Valentin, L. Savio, "*Formation of diphenyl-bipyridine units by surface assisted cross coupling in Pd-cyclometalled complexes*", **Applied Surface Science**, 2023, 609, 155307.

19 – E. Bianchetti, **D. Perilli**, C. Di Valentin, C. "*Improving the oxygen evolution reaction on Fe_3O_4 (001) with single-atom catalysts*", **ACS Catalysis**, 2023, 13(7), 4811-4823.

20 – R. Breglia, **D. Perilli**, C. Di Valentin, "*Exploring spin states by hybrid functional methods to define correct trends in electrocatalytic activity of SACs embedded in N-doped graphene*",

Materials Today Chemistry, 2023, 33, 101728.

21 – V. Bellotti, C. Daldossi, **D. Perilli**, M. D'Arienzo, M. Stredansky, C. Di Valentin, R. Simonutti "*Mechanism of sustainable photocatalysis based on doped-titanium dioxide nanoparticles for UV to visible light induced PET-RAFT photo-polymerization*", **Journal of Catalysis**, 2023, 428, 115074.

22 – C. Daldossi, **D. Perilli**, L. Ferraro, C. Di Valentin, "*Functionalizing TiO_2 Nanoparticles with Fluorescent Cyanine Dye for Photodynamic Therapy and Bioimaging: A DFT and TDDFT Study*", **The Journal of Physical Chemistry C**, 2024, 128, 2978-2989.

23 – I. Cojocariu, **D. Perilli**, V. Feyer, M. Jugovac, "*Graphene-Molecule Hybridization at a Ferromagnetic Interface*", **Chemistry‐A European Journal**, 2024, e202400857.

24 – S. Patil, **D. Perilli**, M. Panighel, A. Baby, C. Cepek, G. Comelli, C. Di Valentin, C. Africh, "*A novel synthesis route with large-scale sublattice asymmetry in boron doped graphene on Ni (111)*", **Surfaces and Interfaces**, 2024, 51, 104700.

25 – G. Carraro, S. E. Atakoohi, **D. Perilli**, O. Alayan, G. Bracco, G. Garbarino, P. M. Leidinger, Z. Novotny, M. Rocca, L. Savio, M. Smerieri, C. Di Valentin, L. Vattuone, "*Hydrogenation of graphene on Ni(111) by H_2 under near ambient pressure conditions*", **Materials Today Chemistry**, 2024, 42, 102359.

26 – V. Chesnyak, **D. Perilli**, M. Panighel, A. Namar, A. Markevich, T. A. Bui, A. Ugolotti, A. Farooq, M. Stredansky, C. Kofler, C. Cepek, G. Comelli, J. Kotakoski, C. Di Valentin, C. Africh, "*Scalable Bottom-up Synthesis of Co-Ni-Doped Graphene*", **Science Advances**, 2024, 10, eado8956.

27 – **D. Perilli**, S. Freddi, M. Zanotti, G. Drera, A. Casotto, S Pagliara, L. Sangaletti, C. Di Valentin, "*Design of highly responsive chemiresistor-based sensors by interfacing NiPc with graphene*", **Communications Materials**, 2024, 5, 254.

28 – X. Shi, H. Liu, Y. Zhang, **D. Perilli**, D. Karpinski, Y. Guo, J. Zhao, J. Gao, "*MXene Manipulating the Electronic and Photoelectric Properties of a Fullerene-Layered Heterojunction*", **The Journal of Physical Chemistry Letters**, 2024, 15, 11911-11918.

29 – **D. Perilli**, V. Chesnyak, A. Ugolotti, M. Panighel, S. Vigneri, F. Armillotta, P. Naderasli, M. Stredansky, M. Schied, P. Lacovig, S. Lizzit, C. Cepek, G. Comelli, H. Brune, C. Africh, C. Di Valentin, "*CO Adsorption on a Single-Atom Catalyst Stably Embedded in Graphene*". **Angewandte Chemie International Edition**, 2025, e202421757.

LIST OF CONFERENCES, WORKSHOPS AND SEMINARS CONTRIBUTIONS

POSTER

1. **2nd World Congress and EXPO on Graphene & 2D Materials**, Frankfurt (Germany), November 6-7, 2017 (poster presentation)
2. **Graphene 2018**, Dresden (Germany), June 26-29, 2018 (poster presentation)
3. **Learn About How Quantum Mechanical Simulations Can Elevate the Design of Materials**, Darmstadt (Germany), October 23, 2018
4. **Graphene Week 2019**, Helsinki (Finland), September 23-27, 2019 (poster presentation)
5. **Materials Day 2022: Simulation and Modeling of Extended Materials – Connecting Scales for Practical Applications**, online workshop, October 14, 2022 (poster contribution)

ORAL

1. **EMRS 2021 Fall Meeting**, online conference, September 20-23, 2021 (oral contribution)
2. **Trends in Nanostructured Carbon Materials and Devices**, online workshop, January 28, 2022 (invited oral presentation)
3. **ECOSS35**, Belval Campus (Luxembourg), August 29 - September 2, 2022 (oral contribution)
4. **From Surfaces to Devices: Novel Perspectives from Nanostructured Oxides and Carbon Materials**, Brescia (Italy), December 12, 2022 (invited oral presentation)
5. **CMD30 FisMat 2023**, Milan (Italy), September 4-8, 2023 (oral contribution)
6. **Invited Seminar at the Department of Physics, Dalian University of Technology**, Dalian (China), September 4-8, 2023 (invited oral presentation)
7. **NanoSEA 2024**, Marseille (France), July 16-19, 2024 (oral contribution)
8. **EMRS 2024 Fall Meeting**, Warsaw (Poland), September 16-19, 2024 (oral contribution)

SKILLS & LANGUAGES

- Electronic structure calculations using density functional theory (DFT) methods for nanostructured materials in electrocatalytic and sensing devices, employing both localized atomic bases and plane waves.
- Strong ability to work in teams.
- Supervision of undergraduate and master's students and PhD candidates.
- Familiarity with Unix environments and shell commands.
- Proficient in Microsoft Office™ suite (Word™, PowerPoint™, Excel™).
- Strong knowledge of graphics software (GIMP, ChemDraw, Xmgrace, Gwyddion, Gnuplot).
- Basic programming knowledge (Python) and experience with HPC environments.

- Proficiency in computational chemistry software and codes using atomic basis sets and plane waves (QuantumEspresso, GAUSSIAN, CRYSTAL, VMD, VESTA, xCrySDen, Jmol, MOLDEN, ASE).
- Languages: Italian (native), English (fluent, written and spoken), Spanish (basic, written and spoken).