►PERSONAL INFORMATION

Name: Dr. Giovanni DI LIBERTO
Date of Birth: 13 April 1991
Age: 31 years old
Nationality: Italian

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►RESEARCH INTERESTS

Computational electro- and photo-catalysis; theoretical chemistry; Density Functional Theory; ab-initio molecular dynamics; materials science; interfaces; heterogeneous catalysis.

►CURRENT POSITIONS

2020-today: Assistant Professor (RTDa) in Inorganic Chemistry (CHIM/03), Department of Materials Science, University of Milan-Bicocca (Italy).

►PREVIOUS POSITIONS

2019-2019: Visiting Scientist at the Universitat de Barcelona (Spain), Laboratory of Prof. Francesc Illas.

2018-2020: Postdoctoral fellow at the University of Milan-Bicocca (Italy), Laboratory of Prof. Gianfranco Pacchioni.

EDUCATION

2019: PhD in Chemical Sciences, University of Milan (Italy), Thesis title: “New Semiclassical Theories for Vibrational Spectroscopy”. Supervisor: Prof. Michele Ceotto.

2015: MSc in Chemical Sciences (110/110 cum laude, highest grade), University of Milan (Italy).

►HONORS AND ACCOLLADES

2022: “Gianpaolo Brivio” International award for the physics and chemistry of Materials.

2022: National Scientific Habilitation as Associate Professor in the sectors of Physical Chemistry (03/A2) and Inorganic Chemistry (03/B1).

2020: “Giuseppe Del Re” award from the Division of Theoretical and Computational Chemistry of the Italian Chemical Society.

2019: “Giovani Talenti” award from University of Milan-Bicocca and Accademia Nazionale dei Lincei.

2018: “Young Physical Chemist” award from the Division of Physical Chemistry of the Italian Chemical Society.

2014: “Italo Martina” degree award from Rotary Club Milano Duomo, Rotary International.

►TEACHING ACTIVITY: LECTURER

2022-today: Lecturer for “General Chemistry”, University of Milan-Bicocca (Italy) (Undergraduate, 2 ECTS, 150 students).

2020-today: Lecturer for the “Laboratory of General and Inorganic Chemistry”, University of Milan-Bicocca (Italy) (Undergraduate, 4 ECTS, 40 students).

2020: Teaching assistant for “Chemistry of Inorganic Materials” (Undergraduate, 6 ECTS, Lecturer: Prof. Gianfranco Pacchioni), University of Milan-Bicocca (Italy).

2018: Teaching assistant for “Physical Chemistry A” (Graduate, 6 ECTS, Lecturer: Prof. Michele Ceotto), University of Milan (Italy).

►TEACHING ACTIVITY: SUPERVISION OF YOUNG STUDENTS AND POST-DOCS

2021: Co-supervisor of 1 MSc student at the University of Pisa, which was visiting student at the University of Milan-Bicocca.

2019-today:
Co-supervisor of a MSc student in Physics at University of Milan-Bicocca. Co-supervisor of 8 BSc students at University of Milan-Bicocca. One of them is current a PhD student at the Universidad de Barcelona in the field of Computational Chemistry.

2019-2022: Co-supervisor of a PhD student at the University of Milan-Bicocca.

►INSTITUTIONAL RESPONSIBILITIES

2022-today: Head Mentor for Lombardian finalists of the national competition “*Giochi della Chimica*”.
2022-today: Dean of the activity “*Giochi della Chimica*” with the Chemical Science teaching committee of the University of Milan Bicocca.

►REVIEWING AND EDITORIAL ACTIVITIES

2022-today: Member of the Editorial Board of Frontiers in Catalysis as Review Editor.

2020-today: Topic Editor of Materials (IF=3.5).

2018-today: Reviewer for *Nature Review Chemistry*, *Angewandte Chemie*, *ACS Catalysis*, *Small, Chemical Science, Applied Surface Science, Catalysis Science & Technology, Solar Energy, Journal of Physical Chemistry C, Physical Chemistry Chemical Physics* & others (reviewing >15 papers/year).

►PEER-REVIEWED PROJECTS

2022: PI of the ISCRA B project “OER-SACs” funded by CINECA entitled “Modelling Oxygen Evolution Reaction on Dry and Wet Single Atom Catalysts”.

2021: PI of the ISCRA B project “GCN-WET” funded by CINECA entitled “Modelling dry and wet g-C_3N_4 based Heterojunctions with Efficient Band Edges Alignment and Photoactivity”.

2020: PI of the ISCRA B project “TT-LSEMI” funded by CINECA entitled “Modelling TiO_2-Passivated Low Band Gap Semiconductors for Efficient Electron Injection and High Photoactivity”.

2019: PI of the “HPC17W04A2” project funded by HPC Europa3 entitled “Modelling of realistic TiO_2-based heterojunctions by means of Density Functional Theory”. The project included two month as visiting scientist at Universidad de Barcelona.

2019: PI of the ISCRA B project “THETEC” funded by CINECA entitled “Modelling of a TiO_2 (001)-(101) based heterojunction with an efficient charge carrier separation and high photoactivity”.

►BIBLIOMETRIC RECORD

51 papers, 24 as first author, 16 as corresponding author, 36 without my PhD supervisor. The works have received around 800 citations, see Scopus, with an H-index of 19, and an average citation per paper of 16. Three journal front cover (1 *Chem Sci*, 1 in *J. Mater. Chem. A*, and 1 in *Chem. Eur. J.*).

► INVITED TALKS

2022: “Role of Dihydrogen Complexes in Hydrogen Evolution Reaction on Single Atom Catalysts” European Conference of Surface Science (ECOSS).

2022: “Rational Design of Semiconductor Interfaces for Photocatalysis” National Meeting of the Division of Theoretical and Computational Chemistry of the Italian Chemical Society.

2022: “Role of Dihydrogen Complexes in Hydrogen Evolution Reaction on Single Atom Catalysts” COST workshop. “Computational water splitting, where we are now and where to go?

2020: "Theoretical Description of BiVO4- based Heterojunctions for Photocatalytic Water Splitting: Insights from DFT", COST workshop, CA18234. Computational materials sciences for efficient water splitting with nanocrystals from abundant elements. First International Symposium on the DFT Modelling of Materials Relevant for Water Splitting.

2021: “Rational Design of Semiconductors Interfaces for Photocatalysis" Conference of the Italian Chemical Society.

2018: Seminar at the Universidad de Barcelona related to the modelling od advanced photocatalysts.

Scientific publications (20 top publications)

1. G. Vilé*****, **G. Di Liberto**, S. Tosoni, A. Sivo, V. Ruta, M. Nachtegaal, A. Clark, S. Agnoli, Y. Zou, A. Savateev, M. Antonietti, G. Pacchioni "Azide-alkyne click chemistry over a heterogeneous copper-based single-atom catalyst" *ACS Catal.* **2022**, *12*, 2947.

2. M.A. Bajada, J. Sanjosé-Orduna, **G. Di Liberto**, S. Tosoni, G. Pacchioni, T. Noël, and G. Vilé*****, O. Fatale and G. Pacchioni, Interfacing single-atom catalysis with continuous-flow organic electrosynthesis *Chem. Soc. Rev* **2022**, *51*, 3898.

3. **G. Di Liberto***, A. Morales and S. Bromley* An unconstrained approach to systematic structural and energetic screening of materials interfaces, *Nat. Comm.* **2022**, *13*, 1.

4. D. Van Dao, **G. Di Liberto**, D. Y. Shin, H. Ko, J. Park, W. Wang, Q.V. Le, T. Van Nguyen, G. Pacchioni*, I.H. Lee*, LaFeO3 meets nitrogen-doped graphene functionalized with ultralow Pt loading in an impactful Z-scheme flatform for photocatalytic hydrogen evolution, *J. Mater. Chem. A* **2022**, *10*.

5. L.A. Cipriano, **G. Di Liberto*** and G. Pacchioni, Superoxo and Peroxo Complexes on Single-Atom Catalysts: Impact on the Oxygen Evolution Reaction, *ACS Catalysis* **2022**, *19*, 11682.

6. **G. Di Liberto**, L.A. Cipriano and G. Pacchioni*, Role of Dihydride and Dihydrogen Complexes in Hydrogen Evolution Reaction on Single-Atom Catalysts *J. Am. Chem. Soc.* **2021**, *143*, 20431.

7. **G. Di Liberto***, and G. Pacchioni, Band offset in semiconductor heterojunctions *J. Phys. Condens. Matt.* **2021**, *33*, 415002.

8. **G. Di Liberto**, S. Tosoni and G. Pacchioni*, Nature and Role of Surface Junctions in $BiOIO_3$ Photocatalysts *Adv. Funct. Mater.* **2021**, *31*, 2009472.

9. **G. Di Liberto**, L.A. Cipriano, S. Tosoni and G. Pacchioni*, Rational Design of Semiconductor Heterojunctions for Photocatalysis. *Chem. Eur. J.* **2021**, *27*, 13306. "Showcase of outstanding Review-type articles".

10. **G. Di Liberto***, S. Tosoni and G. Pacchioni, Z-Scheme versus type-II junction in gC_3N_4/TiO_2 and $gC_3N_4/SrTiO_3/TiO_2$ heterostructures *Catal. Sci. Technol.* **2021**, *11*, 3589.

11. D. Van Dao, L.A. Cipriano, **G. Di Liberto** et al, Plasmonic Au nanoclusters dispersed in nitrogen-doped graphene as a robust photocatalyst for light-to-hydrogen conversion *J. Mater. Chem. A*. **2021**, *9*, 22810. (Front Cover)

12. L. Lo Presti, V. Pifferi, **G. Di Liberto**, G. Cappelletti, L. Falciola, G. Cerrato, and M. Ceotto*, Direct measurement and modeling of spontaneous charge migration across anatase–brookite nanoheterojunctions *J. Mater. Chem. A.* **2021**, *9*, 7782.

13. **G. Di Liberto***, S. Tosoni, F. Illas and G. Pacchioni, Nature of $SrTiO_3/TiO_2$ (anatase) heterostructure from hybrid density functional theory calculations, *J. Chem. Phys.* **2020**, *152*, 184704.

14. L.A Cipriano, **G. Di Liberto***, S. Tosoni and G. Pacchioni, Quantum confinement in group III– V semiconductor 2D nanostructures, *Nanoscale* **2020**, *12*, 17494.

15. **G. Di Liberto***, S. Tosoni and G. Pacchioni, Role of Heterojunction in Charge Carriers Separation in Coexposed Anatase (001)-(101) Surfaces, *J. Phys. Chem. Lett.* **2019**, *10*, 2372.

16. F. Gabas, **G. Di Liberto**, R. Conte*, M. Ceotto*, Protonated glycine supramolecular systems: the need for quantum dynamics *Chem. Sci.* **2018**, *9*, 7894. 'Pick of the Week' and front cover.

17. **G. Di Liberto**, V. Pifferi, L. Lo Presti*, M. Ceotto*, and L. Falciola*, Atomistic Explanation for Interlayer Charge Transfer in Metal–Semiconductor Nanocomposites: The Case of Silver and Anatase *J. Phys. Chem. Lett.* **2017**, *8*, 5372.

18. M. Ceotto*, **G. Di Liberto**, and R. Conte, Semiclassical "Divide-and-Conquer" Method for Spectroscopic Calculations of High Dimensional Molecular Systems *Phys. Rev. Lett.* **2017**, *119*, 010401.

19. **G. Di Liberto** and M. Ceotto*, The importance of the pre-exponential factor in semiclassical molecular dynamics *J. Chem. Phys.* **2016**, *145*, 144107.

20. D. Meroni*, L. Lo Presti, **G. Di Liberto**, M. Ceotto, R. G. Acres, K. L. Prince, R. Bellani, G. Soliveri and Silvia Ardizzone, A Close Look at the Structure of the TiO_2-APTES Interface in Hybrid Nanomaterials and Its Degradation Pathway: An Experimental and Theoretical Study *J. Phys. Chem. C* **2016**, *121*, 430.