



TO MAGNIFICO RETTORE OF UNIVERSITA' DEGLI STUDI DI MILANO

ID CODE 6408

I the undersigned asks to participate in the public selection, for qualifications and examinations, for the awarding of a type B fellowship at **Dipartimento di Chimica**

Scientist- in - charge: Prof. Alberto Villa

[Ilaria Barlocco]

## CURRICULUM VITAE

### PERSONAL INFORMATION

Surname	Barlocco
Name	Ilaria

### PRESENT OCCUPATION

Appointment	Structure
Research fellow	Università di Milano Bicocca

### EDUCATION AND TRAINING

Degree	Course of studies	University	year of achievement of the degree
Degree	Scienze Chimiche	Università degli Studi di Milano	2017
PhD	Chemistry	Università degli Studi di Milano	2022

### FOREIGN LANGUAGES

Languages	level of knowledge
English	C1
Spanish	B1



## AWARDS, ACKNOWLEDGEMENTS, SCHOLARSHIPS

Year	Description of award
2023	Premio GIC (Società Chimica Italiana, Gruppo di Catalisi) Miglior Tesi di Dottorato nel campo della catalisi (Italian Chemical Society - GIC Award Best PhD Thesis in the field of catalysis)
2023	Premio Giovani Talenti dell'Università degli Studi di Milano Bicocca
2023	Borsa per la partecipazione al Congresso DCTC2023 (Scholarship for attending the DCTC2023 congress of SCI - Computational Chemistry division)
2019	3 months Erasmus+ Scholarship
2018	5 months Erasmus+ Scholarship

## TRAINING OR RESEARCH ACTIVITY

description of activity
<p><b>Research Fellow: 2022 - present, Università degli Studi di Milano Bicocca. Supervisor: Prof. Gianfranco Pacchioni. (Cariplo project CO2EnRich).</b></p> <p>Simulation of innovative materials for i) water splitting, focusing on the structural and electronic properties of Single Atom Catalysts (SACs) ii) CO<sub>2</sub> activation and conversion (Cariplo project CO2EnRich), studying non-noble metals supported on oxides of different nature.</p>
<p><b>Visiting Scientist: May 1st 2019 - August 1st 2019, Cardiff University. Supervisor: Dr. Alberto Roldan Martinez</b></p> <p>Simulation of the structural and electronic properties using DFT of graphitic surfaces, Pd, AuPd and Au nanoparticles supported on carbonaceous materials for the production of hydrogen from liquid hydrogen carriers.</p>
<p><b>Ph.D Candidate: 2018 - 2021, Università degli Studi di Milano. Supervisor: Prof. Alberto Villa. Thesis title: Hydrogen production from chemical hydrogen storage materials using carbon-based catalysts.</b></p> <p>Production of hydrogen from the decomposition of liquid carriers, i.e. formic acid and hydrazine, tuning Pd-based heterogeneous catalysts (especially PdAu and PdRh catalysts). Synthesis and advanced characterization of supported heterogeneous catalysts and carbocatalysts with different structural and electronic properties. Evaluation of the prepared catalysts in batch and fixed bed reactors.</p>
<p><b>Visiting Scientist: March 1st 2018 - August 1st 2018, Universidad de Granada. Supervisor: Prof. Francisco H. Maldonado Hodar.</b></p> <p>Synthesis and characterization of different carbon xerogel tested in different gas phase reactions.</p>
<p><b>Stage: January 7th 2018 - February 28th 2018, Università degli Studi di Milano. Supervisor: Prof. Laura Prati.</b></p> <p>Test of Au-based heterogeneous catalysts in the oxidation of glycerol.</p>

## PROJECT ACTIVITY

Year	Project
2022	ISCRA C project: Modelling water splitting reaction on single atom catalysts using covalent organic frameworks as support (SACsCOF) 24 000 h on M100.



## CONGRESSES AND SEMINARS

Date	Title	Place
September 2023	DCTC 2023	Pisa (Italy)
September 2021	SCI 2021	Webinar
April 2021	RENews: Hydrogen	Webinar
February 2020	Sinchem winter school	Bologna (Italy)

## PUBLICATIONS

Articles in reviews
<p>1) Barlocco, Iliaria, Di Liberto, Giovanni, Pacchioni, Gianfranco. "New Scaling Relationships for the Oxygen Evolution Reaction on Single Atom Catalysts." <i>Catalysis Today</i>, 427 (October 2023): 114409. <a href="https://doi.org/10.1016/j.cattod.2023.114409">https://doi.org/10.1016/j.cattod.2023.114409</a> (Research grants)</p> <p>2) Barlocco, Iliaria, Di Liberto, Giovanni, Pacchioni, Gianfranco. "Hydrogen complexes on single atom alloys: classical chemisorption versus coordination chemistry." <i>Catal. Sci. Technol</i> 13, 18 (August 2023): 5301-5312. <a href="https://doi.org/10.1039/D3CY00609C">https://doi.org/10.1039/D3CY00609C</a> (Research grants)</p> <p>3) Di Liberto, Giovanni, Barlocco, Iliaria, Giordano, Livia, Tosoni, Sergio, Pacchioni, Gianfranco. "Single-atom electrocatalysis from first principles: Current status and open challenges." <i>Current Opinion in Electrochemistry</i> 40 (June 2023): 101343. <a href="https://doi.org/10.1016/j.coelec.2023.101343">https://doi.org/10.1016/j.coelec.2023.101343</a> (Research grants)</p> <p>4) Barlocco, Iliaria, Maleki, Farahnaz, Pacchioni, Gianfranco. "CO<sub>2</sub> activation on Cu/TiO<sub>2</sub> nanostructures: importance of dual binding site" <i>Chem. Eur. J.</i> 29, 33 (April 2023): e202300757. <a href="https://doi.org/10.1002/chem.202300757">https://doi.org/10.1002/chem.202300757</a> (Research grants)</p> <p>5) Barlocco, Iliaria, Di Liberto, Giovanni, Pacchioni, Gianfranco. "Hydrogen and oxygen evolution reactions on single atom catalysts stabilized by a covalent organic framework." <i>Energy Adv.</i> 2 (May 2023): 1022-1029. 10.1039/D3YA00162H (Research grants)</p> <p>6) Xiaohui, Wang, Barlocco, Iliaria, Capelli, Villa, Alberto, Kubel, Christian, Huang, Di. "Disclosing the Leaching Behavior of Pd@CMK3 catalysts in Formic Acid Decomposition by Electron Tomography." <i>Nanoscale Adv.</i> 5, 4 (January 2023): 1141-1151. 10.1039/D2NA00664B (PhD Thesis)</p> <p>7) Barlocco, Iliaria, Cipriano, Luis Antonio, Di Liberto, Giovanni, Pacchioni, Gianfranco. "Does the Oxygen Evolution Reaction Follow the Classical OH*, O*, OOH* Path on Single Atom Catalysts?" <i>J. Catal.</i> 417 (January 2023): 351-359. <a href="https://doi.org/10.1016/j.jcat.2022.12.014">https://doi.org/10.1016/j.jcat.2022.12.014</a> (Research grants)</p> <p>8) Bellomi, Silvio, Barlocco, Iliaria, Chen, Xiaowei, Delgado, Juan J., Arrigo, Rosa, Dimitratos, Nikolaos, Roldan, Alberto, Villa, Alberto. "Enhanced stability of sub-nanometric iridium decorated graphitic carbon nitride for H<sub>2</sub> production upon hydrous hydrazine decomposition." <i>Phys. Chem. Chem. Phys.</i> 25, 2 (November 2022): 1081-1095. 10.1039/D2CP04387D (PhD Thesis)</p> <p>9) Barlocco, Iliaria, Cipriano, Luis Antonio, Di Liberto, Giovanni, Pacchioni, Gianfranco. "Modeling Hydrogen and Oxygen Evolution Reactions on Single Atom Catalysts with Density Functional Theory: Role of the Functional." <i>Adv. Theory Simul.</i> (September 2022): 2200513. <a href="https://doi.org/10.1002/adts.202200513">https://doi.org/10.1002/adts.202200513</a> (Research grants)</p> <p>10) Campisi, Sebastiano, Motta, Davide, Barlocco, Iliaria, Stones, Rebecca, Chamberlain, Thomas W., Arunabhiram, Chutia, Dimitratos, Nikolaos, Villa, Alberto. "Furfural Adsorption and Hydrogenation at the Oxide-Metal Interface:</p>



Evidence of the Support Influence on the Selectivity of Iridium-Based Catalysts." ChemCatChem, 14 (March 2022): e202101700. <https://doi.org/10.1002/cctc.202101700> (Research grants)

11) Barlocco, Ilaria, Bellomi, Silvio, Tumiatì, Simone, Fumagalli, Patrizia, Dimitratos, Nikolaos, Roldan, Alberto, Villa, Alberto. "Selective decomposition of hydrazine over metal free carbonaceous materials." Phys. Chem. Chem. Phys., 24 (January 2022): 3017-3029. <https://doi.org/10.1039/D1CP05179B> (PhD Thesis)

12) Barlocco, Ilaria, Bellomi, Silvio, Delgado, Juan J., Chen, Xiaowei, Prati, Laura, Dimitratos, Nikolaos, Roldan, Alberto, Villa, Alberto. "Enhancing activity, selectivity and stability of palladium catalysts in formic acid decomposition: Effect of support functionalization." Catalysis Today, 382 (December 2021): 61-70. <https://doi.org/10.1016/j.cattod.2021.07.005> (PhD Thesis)

13) Capelli, Sofia, Barlocco, Ilaria, Scesa, Federico M., Huang, Xiaohui, Wang, Di, Tessore, Francesca, Villa, Alberto, Di Michele, Alessandro, Pirola, Carlo. "Pd-Au Bimetallic Catalysts for the Hydrogenation of Muconic Acid to Bio-Adipic Acid." Catalysts, 11, 11 (October 2021): 1313. <https://doi.org/10.3390/catal11111313> (Collaborations)

14) Barlocco, Ilaria, Capelli, Sofia, Lu, Xiuyuan, Bellomi, Silvio, Huang, Xiaohui, Wang, Di, Prati, Laura, Dimitratos, Nikolaos, Roldan, Alberto, Villa, Alberto. "Disclosing the Role of Gold on Palladium-Gold Alloyed Supported Catalysts in Formic Acid Decomposition." ChemCatChem, 13, 19 (October 2021): 4210-4222. <https://doi.org/10.1002/cctc.202100886> (PhD Thesis)

15) Hafeez, Sanaa, Barlocco, Ilaria, Al-Salem, Sultan M., Villa, Alberto, Chen, Xiaowei, Delgado, Juan J., Manos, George, Dimitratos, Nikolaos, Constantinou, Achilleas. "Experimental and process modelling investigation of the hydrogen generation from formic acid decomposition using a Pd/Zn catalyst." Appl. Sci., 11, 18 (September 2021): 8462. <https://doi.org/10.3390/app11188462> (PhD Thesis)

16) Motta, Davide, Barlocco, Ilaria, Bellomi, Silvio, Villa, Alberto, Dimitratos, Nikolaos. "Hydrous Hydrazine Decomposition for Hydrogen Production Using of Ir/CeO<sub>2</sub>: Effect of Reaction Parameters on the Activity." Nanomaterials, 11, 5 (May 2021): 1340. <https://doi.org/10.3390/nano11051340> (PhD Thesis)

17) Dogra, Ashima, Sharma, Vinit, Barlocco, Ilaria, Villa, Alberto, Gupta, Neeraj. "A proof of concept for cooperation from the quinone groups adjacent to N sites during the metal-free oxidation of glycerol by nitrogen-rich graphene oxide." New J. Chem., 45, 42 (October 2021): 19651-19654. <https://doi.org/10.1039/D1NJ04226B> (Collaborations)

18) Barlocco, Ilaria, Capelli, Sofia, Zanella, Elisa, Chen, Xiaowei, Delgado, Juan J., Roldan, Alberto, Dimitratos, Nikolaos, Villa, Alberto. "Synthesis of palladium-rhodium bimetallic nanoparticles for formic acid dehydrogenation." J. Energy Chem., 52 (January 2021): 301-309. <https://doi.org/10.1016/j.jechem.2020.04.031> (PhD Thesis)

19) Barlocco, Ilaria, Capelli, Sofia, Lu, Xiuyuan, Tumiatì, Simone, Dimitratos, Nikolaos, Roldan, Alberto, Villa, Alberto. "Role of defects in carbon materials during metal-free formic acid." Nanoscale, 12, 44 (October 2020): 22768-22777. <https://doi.org/10.1039/D0NR05774F> (PhD Thesis)

20) Dogra, Ashima, Barlocco, Ilaria, Singh, Amritpal, Somodi, Ferenc, Villa, Alberto, Gupta, Neeraj. "Metal free alkene hydrogenation by B-doped graphitic carbon nitride." Catal. Sci. Technol. 10, 9 (April 2020): 3024-3028. <https://doi.org/10.1039/D0CY00488J> (Collaborations)

21) Jouve, Andrea, Stucchi, Marta, Barlocco, Ilaria, Evangelisti, Claudio, Somodic, Ferenc, Villa, Alberto, Prati, Laura. "Carbon-supported Au nanoparticles: catalytic activity ruled out by carbon support." Top. Catal., 61, 18 (November 2018): 1928-1938. <https://doi.org/10.1007/s11244-018-1001-7> (Collaborations)

## Congress proceedings

Oral Communication - "Does the Oxygen Evolution Reaction follow the classical OH\*, O\*, OOH\* path on single atom catalysts?" DCTC 2023, Pisa (Italy) September 20th 2023

Oral Communication - "Disclosing the Role of Gold on Palladium - Gold Alloyed Catalysts in Formic Acid Decomposition" SCI 2021, Webinar, September 15th 2021

Oral Communication - "Role of Defects in Metal-Free Formic Acid Dehydrogenation" RENews: Hydrogen, webinar della Società Chimica Italiana, Gruppo EnerCHEM, April 3rd 2021



## OTHER INFORMATION

Teaching
Chimica Generale ed Inorganica (Prof. Sergio Tosoni, 20 h), Laurea in Scienze e tecnologie per l'ambiente (2023).
Supporto alla didattica nell'ambito del progetto SVELAMI-B - SVolgere Esperimenti nei Laboratori di Milano-Bicocca reloaded, interventi volti a favorire l'equilibrio di genere nell'accesso alle diverse aree disciplinari dei corsi di studio (Prof.ssa Livia Giordano, 20 h) (2023).
Chimica Generale ed Inorganica (Dr. Giovanni Di Liberto, 36 h), Laurea triennale in chimica, Università degli studi di Milano Bicocca (2022).
Elementi di chimica analitica strumentale (Prof.ssa Monica Panigati, 32 h), Laurea triennale in scienze farmaceutiche e biomolecolari, Università degli studi di Milano (2019).
Chimica analitica II (Prof. Alberto Villa, 24 h), Laurea triennale in chimica, Università degli studi di Milano (2020).
Chimica analitica II (Prof. Vittoria Guglielmi, 24 h), Laurea triennale in chimica industriale, Università degli studi di Milano (2020).
Chimica analitica II (Prof. Alberto Villa, 24 h), Laurea triennale in chimica, Università degli studi di Milano (2021).
Tutoraggio di studenti delle scuole superiori per preparazione ai "Giochi della chimica" ed. 2019 (16 h).

Declarations given in the present curriculum must be considered released according to art. 46 and 47 of DPR n. 445/2000.

The present curriculum does not contain confidential and legal information according to art. 4, paragraph 1, points d) and e) of D.Lgs. 30.06.2003 n. 196.

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Place and date: Milano, 08/02/2024