



ALLA MAGNIFICA RETTRICE  
DELL'UNIVERSITA' DEGLI STUDI DI MILANO

COD. ID: A011

Il sottoscritto chiede di essere ammesso a partecipare alla selezione pubblica, per titoli ed esami, per il conferimento di un assegno di ricerca presso il Dipartimento di Chimica

Responsabile scientifico: Prof.ssa Laura Prati

[Ilaria Barlocco]

## CURRICULUM VITAE

### INFORMAZIONI PERSONALI

Cognome	Barlocco
Nome	Ilaria

### OCCUPAZIONE ATTUALE

Incarico	Struttura
Research fellow	Università di Milano

### ISTRUZIONE E FORMAZIONE

Titolo	Corso di studi	Università	anno conseguimento titolo
Dottorato Di Ricerca	Chemistry	Università degli Studi di Milano	2022
Laurea Magistrale o equivalente	Scienze Chimiche	Università degli Studi di Milano	2017

### LINGUE STRANIERE CONOSCIUTE

lingue	livello di conoscenza
English	C1
Spanish	B1

### PREMI, RICONOSCIMENTI E BORSE DI STUDIO

anno	Descrizione premio
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

## ATTIVITÀ DI FORMAZIONE O DI RICERCA

descrizione dell'attività
<p><b>Research Fellow: 2024 - now, Università degli Studi di Milano. Supervisor: Prof. Alberto Villa. (<i>Produzione di idrogeno verde da acque reflue ricche di idrazina attraverso nuovi processi catalitici - codice CUP: G53D23003370006</i>)</b></p> <p>Synthesis and characterization of metal based catalysts for i) production of hydrogen from ammonia borane and ii) biomass conversion</p>
<p><b>Research Fellow: 2022 - 2024, 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>

## ATTIVITÀ PROGETTUALE

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



## CONGRESSI, CONVEGNI E SEMINARI

Data	Titolo	Sede
August 2024	SCI 2024	Milan (Italy)
June 2024	CARBOCAT10	Florence (Italy)
September 2023	DCTC 2023	Pisa (Italy)
September 2021	SCI 2021	Webinar
April 2021	RENews: Hydrogen	Webinar
February 2020	Sinchem winter school	Bologna (Italy)

## PUBBLICAZIONI

Articoli su riviste
(1) Barlocco, Ilaria, Cattaneo, Stefano, Bellomi, Silvio, Stucchi, Marta, Pifferi, Valentina, Delgado, Juan J., Chen, Xiaowei, Falciola, Luigi, Prati, Laura, Villa, Alberto. <i>"Influence of the Au-Ag Morphology in the Electrocatalytic Reduction of Organic Halides"</i> Molecular Catalysis, accepted for publication
(2) Bellomi, Silvio, Cano-Blanco, Daniel, Barlocco, Ilaria, Delgado, Juan J., Chen, Xiaowei, Prati, Laura, Ferri, Davide, Dimitratos, Nikolaos, Roldan, Alberto, Villa, Alberto. <i>"Probing the Metal/Oxide Interface of IrCoCeO<sub>x</sub> in N<sub>2</sub>H<sub>4</sub>-H<sub>2</sub>O Decomposition: An Experimental and Computational Study"</i> ACS Appl. Mater. Interfaces, 16, 40 (October 2024) 54897-54906. <a href="https://doi.org/10.1021/acsami.4c12306">https://doi.org/10.1021/acsami.4c12306</a>
(3) Stucchi, Marta, Barlocco, Ilaria, Villa, Alberto, Pifferi, Valentina, Falciola, Luigi, Prati, Laura. <i>"Studying the formation and the final structure of AuPt bimetallic systems by cyclic voltammetry"</i> Arkivoc, 2024, 3 (September 2024) <a href="https://doi.org/10.24820/ark.5550190.p012.258">https://doi.org/10.24820/ark.5550190.p012.258</a>
(4) Barlocco, Ilaria, Spotti, Matteo, Di Liberto, Giovanni, Pacchioni, Gianfranco. <i>"Electrochemical Nitrogen Reduction Reaction from Ab Initio Thermodynamics: Single versus Dual Atom Catalysts"</i> Advanced Theory and Simulations, 7, 9 (July 2024): 2400536. <a href="https://doi.org/10.1002/adts.202400536">https://doi.org/10.1002/adts.202400536</a>
(5) Zanella, Elisa, Franchi, Stefano, Jabbarli, Narmin, Barlocco, Ilaria, Stucchi, Marta, Pirola, Carlo. <i>"Effect of Support Functionalization on Catalytic Direct Hydrogenation and Catalytic Transfer Hydrogenation of Muconic Acid to Adipic Acid"</i> Catalysts, 14, 7 (July 2024): 465. <a href="https://doi.org/10.3390/catal14070465">https://doi.org/10.3390/catal14070465</a>
(6) Saetta, Clara, Barlocco, Ilaria, Di Liberto, Giovanni, Pacchioni, Gianfranco. <i>"Key Ingredients for the Screening of Single Atom Catalysts for the Hydrogen Evolution Reaction: The Case of Titanium Nitride"</i> Small, 20, 37 (April 2024): 2401058. <a href="https://doi.org/10.1002/sml.202401058">https://doi.org/10.1002/sml.202401058</a>
(7) Gupta, Neeraj, Barlocco, Ilaria, Khavryuchenko, Oleksiy, Villa, Alberto. <i>"Metal-Free Catalytic Conversion of Veratryl and Benzyl Alcohols through Nitrogen-Enriched Carbon Nanotubes"</i> C-Journal of Carbon Research, 10, 1 (March 2024): 13. <a href="https://doi.org/10.3390/c10010013">https://doi.org/10.3390/c10010013</a>
(8) Hafeez, Sanaa, Harkou, Eleana, Adamou, Panayiota, Barlocco, Ilaria, Zanella, Elisa, Manos, George, Al-Salem, Sultan, Chen, Xiaowei, Delgado, Juan José, Dimitratos, Nikolaos, Villa, Alberto, Constantinou,



Achilleas. "Formic Acid Decomposition Using Palladium-Zinc Preformed Colloidal Nanoparticles Supported on Carbon Nanofibre in Batch and Continuous Flow Reactors: Experimental and Computational Fluid Dynamics Modelling Studies" <i>Nanomaterials</i> , 13, 23 (December 2023): 2993. <a href="https://doi.org/10.3390/nano13232993">https://doi.org/10.3390/nano13232993</a>
(9) Barlocco, Ilaria, 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>
(10) Bellomi, Silvio, Barlocco, Ilaria, Tumiat, Simone, Fumagalli, Patrizia, Dimitratos, Nikolaos, Roldan, Alberto, Villa, Alberto. "Effects of oxygen functionalities on hydrous hydrazine decomposition over carbonaceous materials" <i>Dalton Transactions</i> , 52,43 (September 2023): 15871-15877. <a href="https://doi.org/10.1039/D3DT02310A">https://doi.org/10.1039/D3DT02310A</a>
(11) Barlocco, Ilaria, 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>
(12) Di Liberto, Giovanni, Barlocco, Ilaria, 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>
(13) Barlocco, Ilaria, 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>
(14) Barlocco, Ilaria, 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. <a href="https://doi.org/10.1039/D3YA00162H">10.1039/D3YA00162H</a>
(15) Xiaohui, Wang, Barlocco, Ilaria, 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. <a href="https://doi.org/10.1039/D2NA00664B">10.1039/D2NA00664B</a>
(16) Barlocco, Ilaria, 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>
(17) Bellomi, Silvio, Barlocco, Ilaria, 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. <a href="https://doi.org/10.1039/D2CP04387D">10.1039/D2CP04387D</a>
(18) Barlocco, Ilaria, 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>
(19) Campisi, Sebastiano, Motta, Davide, Barlocco, Ilaria, Stones, Rebecca, Chamberlain, Thomas W., Arunabharam, Chutia, Dimitratos, Nikolaos, Villa, Alberto. "Furfural Adsorption and Hydrogenation at the Oxide-Metal Interface: Evidence of the Support Influence on the Selectivity of Iridium-Based Catalysts." <i>ChemCatChem</i> , 14 (March 2022): e202101700. <a href="https://doi.org/10.1002/cctc.202101700">https://doi.org/10.1002/cctc.202101700</a>
(20) Barlocco, Ilaria, Bellomi, Silvio, Tumiat, Simone, Fumagalli, Patrizia, Dimitratos, Nikolaos, Roldan, Alberto, Villa, Alberto. "Selective decomposition of hydrazine over metal free carbonaceous materials." <i>Phys. Chem. Chem. Phys.</i> , 24 (January 2022): 3017-3029. <a href="https://doi.org/10.1039/D1CP05179B">https://doi.org/10.1039/D1CP05179B</a>
(21) 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." <i>Catalysis Today</i> , 382 (December 2021): 61-70. <a href="https://doi.org/10.1016/j.cattod.2021.07.005">https://doi.org/10.1016/j.cattod.2021.07.005</a>
(22) 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." <i>Catalysts</i> , 11, 11 (October 2021): 1313. <a href="https://doi.org/10.3390/catal11111313">https://doi.org/10.3390/catal11111313</a>



(23) 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." <i>ChemCatChem</i> , 13, 19 (October 2021): 4210-4222. <a href="https://doi.org/10.1002/cctc.202100886">https://doi.org/10.1002/cctc.202100886</a>
(24) 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." <i>Appl. Sci.</i> , 11, 18 (September 2021): 8462. <a href="https://doi.org/10.3390/app11188462">https://doi.org/10.3390/app11188462</a>
(25) 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." <i>Nanomaterials</i> , 11, 5 (May 2021): 1340. <a href="https://doi.org/10.3390/nano11051340">https://doi.org/10.3390/nano11051340</a>
(26) 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." <i>New J. Chem.</i> , 45, 42 (October 2021): 19651-19654. <a href="https://doi.org/10.1039/D1NJ04226B">https://doi.org/10.1039/D1NJ04226B</a>
(27) 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." <i>J. Energy Chem.</i> , 52 (January 2021): 301-309. <a href="https://doi.org/10.1016/j.jechem.2020.04.031">https://doi.org/10.1016/j.jechem.2020.04.031</a>
(28) Barlocco, Ilaria, Capelli, Sofia, Lu, Xiuyuan, Tumiat, Simone, Dimitratos, Nikolaos, Roldan, Alberto, Villa, Alberto. "Role of defects in carbon materials during metal-free formic acid." <i>Nanoscale</i> , 12, 44 (October 2020): 22768-22777. <a href="https://doi.org/10.1039/D0NR05774F">https://doi.org/10.1039/D0NR05774F</a>
(29) Dogra, Ashima, Barlocco, Ilaria, Singh, Amritpal, Somodi, Ferenc, Villa, Alberto, Gupta, Neeraj. "Metal free alkene hydrogenation by B-doped graphitic carbon nitride." <i>Catal. Sci. Technol.</i> 10, 9 (April 2020): 3024-3028. <a href="https://doi.org/10.1039/D0CY00488J">https://doi.org/10.1039/D0CY00488J</a>
(30) 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." <i>Top. Catal.</i> , 61, 18 (November 2018): 1928-1938. <a href="https://doi.org/10.1007/s11244-018-1001-7">https://doi.org/10.1007/s11244-018-1001-7</a>

Atti di convegni
Oral Communication - "Does the Oxygen Evolution Reaction follow the classical OH*, O*, OOH* path on single atom catalysts?" SCI 2024, Milan (Italy) August 26 <sup>th</sup> 2024
Short Oral Communication + Poster - "Disclosing the Leaching Behaviour of Pd@CMK <sub>3</sub> Catalysts in Formic Acid Decomposition by Electron Tomography" Carbocat 10, Florence (Italy) June 24 <sup>th</sup> 2024
Oral Communication - "Does the Oxygen Evolution Reaction follow the classical OH*, O*, OOH* path on single atom catalysts?" DCTC 2023, Pisa (Italy) September 20 <sup>th</sup> 2023
Oral Communication - "Disclosing the Role of Gold on Palladium - Gold Alloyed Catalysts in Formic Acid Decomposition" SCI 2021, Webinar, September 15 <sup>th</sup> 2021
Oral Communication - "Role of Defects in Metal-Free Formic Acid Dehydrogenation" RENews: Hydrogen, webinar della Società Chimica Italiana, Gruppo EnerCHEM, April 3 <sup>rd</sup> 2021

## ALTRE INFORMAZIONI

Insegnamenti e tutoraggio
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).

Le dichiarazioni rese nel presente curriculum sono da ritenersi rilasciate ai sensi degli artt. 46 e 47 del DPR n. 445/2000.

Il presente curriculum, non contiene dati sensibili e dati giudiziari di cui all'art. 4, comma 1, lettere d) ed e) del D.Lgs. 30.6.2003 n. 196.

RICORDIAMO che i curricula SARANNO RESI PUBBLICI sul sito di Ateneo e pertanto si prega di non inserire dati sensibili e personali. Il presente modello è già precostruito per soddisfare la necessità di pubblicazione senza dati sensibili.

Si prega pertanto di **NON FIRMARE** il presente modello.

Luogo e data: Milano, 16.12.2024