

CARLO NERVI

Date of Birth: 05/11/1965

Languages: Italian (mother tongue), English (fluent), Russian (Intermediate)

Married with one son.

ORCID, RESEARCHER ID ORCID: 0000-0002-3712-7369, Scopus Author ID: 7006140506 ResearcherID: B-1355-2008

ACADEMIC CAREER

- Master degree in Chemistry (University of Torino), in 1990, 110/110 cum laude.
- PhD in Chemical Sciences (1994, University of Torino).
- Master in "Industrial Electrochemistry" (Palermo 6-10 April 1992)

• "Visiting research fellow" at the Heyrovsky Institute of Physical Chemistry, Academy of Sciences, Czech Republic, (1994, 1998, 2000), working on "Organometallic Electrochemistry" (project COST D5/0008/93 and COST D15/0001/99).

• Researcher at the Department of Chemistry (University of Torino) since 1995.

• "Invited Visiting Professor", at the Department of Chemistry, The University of Montana, Missoula, MT 59812, USA, (2002, semestral course "undergraduate CHEM 455 - Inorganic Chemistry Laboratory").

- Associate Professor since 2010 at the Department of Chemistry, University of Torino, Italy.
- National Habilitation to Full Professor in General and Inorganic Chemistry (03/B1 CHIM/03): 2017

• Visiting Full Professor at Skolkovo Institute of Science and Technology, Moscow, Russia: (December 2023 – April 2024).

• Full Professor at the Skolkovo Institute of Science and Technology, Moscow, Russia (from December 2024).

BIBLIOMETRY Number of pubblications: 132 (scopus 122); h-index: 38 (Scopus) TOTAL NUMBER OF CITATIONS: 4176 (SCOPUS) Google Scholar (<u>https://scholar.google.com/citations?hl=it&user=6vAqf70AAAAJ</u>): h-index 40, 5841 citations Complex Com

He is the author of the computer program ESP (Electrochemical Simulation Package) (developed in C) for electrochemical simulations for research and teaching purposes, and co-author of the book "Inorganic Electrochemistry. Theory, Practice and Application", 2nd Ed., RSC, 2011, ISBN: 978-1-84973-071-6 by Piero Zanello, Fabrizia Fabrizi de Biani, Carlo Nervi.

SELECTED PUBBLICATIONS IN THE FIELD OF ELECTROCHEMICAL REDUCTION OF CO₂

- 1. J.Rongé, T.Bosserez, D.Martel, C.Nervi, L.Boarino, F.Taulelle, G.Decher, S.Bordiga, J.A.Martens, "Monolithic Cells for Solar Fuels", *Chem.Soc.Rev.*, **2014**, *43*, 7963-7981.
- F.Franco, C.Cometto, F.Ferrero Vallana, F.Sordello, E.Priola, C.Minero, C.Nervi, R.Gobetto, "A Local proton source in a [Mn(bpy-R)(CO)₃Br]-type redox catalyst enables CO₂ reduction even in absence of Brønsted acids", *Chem.Commun.*, **2014**, *50*, 14670-14673.
- F.Franco, C.Cometto, C.Garino, C.Minero, F.Sordello, C.Nervi, R.Gobetto, "Photo- and Electrocatalytic Reduction of CO₂ by [Re(CO)₃{α,α'-Diimine-(4-piperidinyl-1,8-naphthalimide)}Cl Complexes", *Eur.J.Inorg.Chem.*, **2015**, 296-304.
- F.Franco, C.Cometto, F.Sordello, C.Minero, L.Nencini, J.Fiedler, R.Gobetto, C.Nervi, "Electrochemical Reduction of CO₂ by M(CO)₄(bpy-type) (M=Mo, W) Complexes: Catalytic Activity Improved by 2,2'-Dipyridylamine", *ChemElectroChem.*, **2015**, *2*, 1372-1379.
- 5. Mukund G. Mali, Hyun Yoon, Bhavana N. Joshi, Hyunwoong Park, Salem S. Al-Deyab, Dong Chan Lim, SeJin Ahn, Carlo Nervi, Sam S. Yoon, "Enhanced Photoelectrochemical Solar Water Splitting Using a Platinum-Decorated CIGS/CdS/ZnO Photocathode", *ACS Appl. Mater. Interfaces*, **2015**, *7*, 21619-21625.

- 6. C.Sun, S.Prosperini, P.Quagliotto, G.Viscardi, S.S.Yoon, R.Gobetto, C.Nervi, "Electrocatalytic Reduction of CO₂ by Thiophene-substituted Rhenium(I) Complexes and by their Polymerized Films", Dalton Trans., 2016, 45.14678-14688.
- 7. C.Sun, R.Gobetto, C.Nervi, "Recent Advances on Catalytic CO₂ Reduction by Organometal Complexes Anchored on Modified Electrodes", New J. Chem., 2016, 40, 5656-5661.
- 8. F.Franco, C.Cometto, L.Nencini, C.Barolo, F.Sordello, C.Minero, J.Fiedler, M.Robert, R.Gobetto, C.Nervi, "Local Proton Source in the Electrocatalytic CO₂ Reduction by Mn(bpy-R)(CO)₃Br Complexes", Chem. Eur. J., 2017, 23, 4782-4793, cover.
- 9. A.Dubey, L.Nencini, R.R.Fayzullin, C.Nervi, J.R.Khusnutdinova, "Bio-Inspired Mn(I) Complexes for the Hydrogenation of CO₂ to Formate and Formamide", ACS Catal., 2017, 7, 3864-3868.
- 10. Laura Rotundo, Claudio Garino, Roberto Gobetto, Carlo Nervi, "Computational Study of the Electrochemical Reduction of W(CO)₄(2,2'-dipyridylamine)", Inorg. Chim. Acta, 2018, 470, 373-378.
- 11. C.Sun, L.Rotundo, C.Garino, L.Nencini, S.S.Yoon, R.Gobetto, C.Nervi, "Electrochemical CO₂ Reduction at Glassy Carbon Electrodes Functionalized by Mn(I) and Re(I) Organometallic Complexes", ChemPysChem, 2017, 18, 3219-3229.
- L.Rotundo, J.Filippi, H.A.Miller, R.Rocca, F.Vizza, R.Gobetto, C.Nervi, "Electrochemical CO₂ reduction in 12. water at carbon cloth electrodes functionalized with a *fac*-Mn(apbpy)(CO)₃Br complex", *Chem.Commun.*, **2019**, 55, 775-777.
- J.Septavaux, C.Tosi, P.Jame, C.Nervi, R.Gobetto, J.Leclaire. "Simultaneous CO₂ capture and metal purification 13. from waste streams using triple-level dynamic combinatorial chemistry", Nature Chem., 2020, https://doi.org/10.1038/s41557-019-0388-5.
- Laura Rotundo, Dmitry E. Polyansky, Roberto Gobetto, David C. Grills, Etsuko Fujita, Carlo Nervi, Gerald F. 14. Manbeck, "Molecular Catalysts with Intramolecular Re-O Bond for Electrochemical Reduction of Carbon Dioxide", Inorg. Chem., 2020, 59, 12187-12199.
- 15. J.Filippi, L.Rotundo, R.Gobetto, H.A.Miller, C.Nervi, A.Lavacchi, F.Vizza, "Turning Manganese into Gold: efficient electrochemical CO₂ reduction by a *fac*-Mn(apbpy)(CO)₃Br complex in a gas-liquid interface flow cell", Chem.Eng.J., 2021, 416, 129050.
- 16. Laura Rotundo, David C. Grills, Dmitry E. Polyansky, Roberto Gobetto, Emanuele Priola, Carlo Nervi, Etsuko Fujita, "Photochemical CO₂ Reduction Using Rhenium(I) Tricarbonyl Complexes with Bipyridyl-Type Ligands with and without Second Coordination Sphere Effects", Chem. Photo. Chem., 2021, 5, 1-13, 10.1002/cptc.202000307
- 17. L.Rotundo, R.Gobetto, C.Nervi, "Electrochemical CO2 reduction with earth-abundant metal catalysts", Curr. Opin. Green Sust. Chem., 2021, 31, 100509, https://doi.org/10.1016/j.cogsc.2021.100509
- 18. F.Marocco Stuardi, A.Tiozzo, L.Rotundo, J.Leclaire, R.Gobetto, C.Nervi, "Efficient Electrochemical Reduction of CO₂ to Formate in Methanol Solutions by Mn Functionalized Electrodes in the Presence of Amines", Chem.Eur.J., 2022, 28(37), e202104377, 1-9, https://doi.org/10.1002/chem.202104377
- L.Rotundo, A.Barbero, C.Nervi, R.Gobetto, "CO2 Electroreduction on Carbon-Based Electrodes 19. Functionalized with Molecular Organometallic Complexes—A Mini Review", Catalysts, 2022, 12, 1448, https://doi.org/10.3390/catal12111448
- 20. Alice Barbero, Laura Rotundo, Chiara Reviglio, Roberto Gobetto, Romana Sokolova, Jan Fiedler, Carlo Nervi, "New Spectroelectrochemical Insights into Manganese and Rhenium Bipyridine Complexes as Catalysts for the Electrochemical Reduction of Carbon Dioxide", Molecules, 2023, 28 (22), 7535, https://doi.org/10.3390/molecules28227535
- 21. Geyla C. Dubed Bandomo, Federico Franco, Changwei Liu, Suvendu Sekhar Mondal, Angelo Gallo, Carlo Nervi, Julio Lloret-Fillol, "Toward the Understanding of the Structure–Activity Correlation in Single-Site Mn Covalent Organic Frameworks for Electrocatalytic CO₂ Reduction", ACS Applied Energy Materials, 2024, https://doi.org/10.1021/acsaem.3c03117
- Elena Andreea Palade, Roberto Gobetto, Carlo Nervi, "Molecular and single-atom catalysts based on earth-22. abundant transition metals for the electroreduction of CO2 to C1", Inorg. Chinm. Acta, 2024, 566, 122029, https://doi.org/10.1016/j.ica.2024.122029
- 23. A. Barbero, F. Pezzano, F. Calderaro, R. Gobetto, C. Reviglio, A. Porceddu, V. Nikitina, J.-F. Li, H. Zhang, Z. Huang, J. Liu, A. Oganov, C. Nervi, "Direct Electrochemical Conversion of Carbon Dioxide into Methanol in Water with High Faradaic Efficiency by Mo-Functionalized Electrode", ChemRxiv, 2024, https://doi.org/10.26434/chemrxiv-22024-26432c26412c.

SCIENTIFIC PROFILE | More than 150 communications to congress. Among them, 14 Invited lectures on the following topics: 1) synthesis and characterization of inorganic and organometallic transition metal complexes (with particular regard to spectroscopic and electrochemical properties and DFT calculation) with potential applications in the field of catalysis and energy materials; 2) use of computational methods (experience with Gaussian, Quantum Espresso, VASP, Gulp, DFTB+, Materials Studio) on molecules and in the solid phase (periodic calculations) as a tool to interpret and predict spectroscopic and reactivity properties (i.e IR, NMR, UV-Vis, electrochemical properties, transition states and reaction mechanisms); 3) use of genetic algorithms (USPEX code) for the in silico prediction of solid structures of molecules and in the field of innovative solid state materials; 4) development and study of Li-ion batteries from both experimental (EIS measurements) and theoretical (ion mobility in solid materials) viewpoints. Scientific attention has been paid to inorganic electrochemistry, but also photoelectrochemistry and artificial photosynthesis, and in recent years with particular attention to the problem of carbon dioxide as starting raw material and its electrochemical reduction. He is co-author, with Piero Zanello and Fabrizia Fabrizi de Biani, of the monograph "Inorganic Electrochemistry. Theory, Practice and Application", 2nd Ed., RSC, 2011, ISBN: 978-1-84973-071-6, which has received 995 citations (google scholar), and author of a computer program (ESP, Electrochemical Simulation Package) for theoretical electrochemistry (Cyclic Voltammetry, Chronoamperometry, polarography and Square Wave Voltammetry) and best fitting of experimental data. The various topics covered have as a common factor electrochemistry (electrocatalysis) and the prediction of properties by means of computational methods.

TEACHING ACTIVITIES

- Stoichiometry for the course "Chemistry" (1st year, Geological Sciences): 1995-1998
- Stoichiometry for the course "Chemistry" (1st year, Natural Sciences): 1996-1999
- Stoichiometry for the course "Chemistry" of Turin Polytechnique, city of Mondovì, (1st year): 1997-1998
- Laboratory of Inorganic Chemistry II (4th year, Chemical Sciences): 1998-1999
- Student training in quantum mechanics and use of CACAO program (Huckel theory) for the course of Inorganic Chemistry II (4th year, Chemical Sciences): 1998-2001
- Assistant for the Laboratory of Inorganic Chemistry I (2nd year, Chemical Sciences): 1998-1999
- Course of General and Inorganic Chemistry with Introduction to Organic Chemistry (1st year, Geological Sciences): 1999-2001
- Course of Laboratory of Inorganic Chemistry II (4th year, Chemical Sciences): 1999-2001
- Course of Chemistry I (1st year, Geological Sciences, 5+1 CFU): 2001-2011
- Course of Computer Sciences for Chemistry (1st year of master degree (laurea specialistica) in Metodologie Chimiche Avanzate, MCA, 3+3 CFU): 2001-2009
- Laboratory of Transition Metal Complexes: synthesis and reactivity (1st year of master degree in MCA, 4+2 CFU): 2001-2009
- Course CHEM 455 of "Inorganic Chemistry Laboratory" (semester) at The University of Montana, Missoula, MT 59812, USA (undergraduate program in Chemistry): 2001-2002
- Course of Electrosynthesis and Electrocatalysis (2nd year of master degree in MCA, 2 CFU):2002-2010
- Course for PhD students (XVIII° ciclo) Biological Active Metal Complexes (3 CFU): 2002-2003
- Course of General and Inorganic Chemistry B (3rd year, Strategical Sciences for military, 3 CFU): 2004-2022
- Course for PhD students (XXII° ciclo) "Metal Complexes in Biology" (4 CFU): 2006-2007
- Course of Inorganic Analysis and Electrochemistry (1st year of master degree Environmental Chemistry 7+3 CFU): 2009-2023
- Course of Catalysis (2nd year, master degree MCA, 6 CFU): 2010-2012
- Course of Applied Electrochemistry: Corrosion and Energy Conversion (master degree, Chemical Sciences 4 CFU): 2011-2016
- Course of Inorganic Chemistry II (3rd year Chemical Sciences, 3+4 CFU):2011-2013
- Course of Laboratory of Organic and Inorganic Chemistry (3rd year Chemistry and Chemical Technology, 1+4 CFU):2013-2014
- Course of Laboratory of Inorganic Syntheses (3rd year Chemistry and Chemical Technology, 1+4 CFU): 2014-2023
- Course of Electrochemistry (4 CFU): 2016-2024
- Course of Laboratory of General and Inorganic Chemistry (2 CFU): 2024

Supervisor and Tutor of 80 undergraduate thesis and 26 master degree thesis.

ACTIVITIES FOR THE DOCTORATE (PHD)

- Tutor of 12 PhD students and panel member and opponent for the assignment of the PhD title for several national and internation universities
- GRANTS AND FOUNDED PROJECTS
- Kao Corporation (Japan): from 2004 to 2007 about 120,000 €/year.
- Project Code A97 "New Anticancer Agents for Use in Neutron Capture Therapy (NCT)" funded by the Piedmont Region (2006-2009) 36000 €
- COST D36-001-06 project "Redox activity of host-guest, organometallic and molecular structures at electrode interfaces" 2006-2011 (coordinator Prof. Lubomir Pospisil, Prague, CZ).
- PHOTORECARB project "Photocatalytic Reduction Of Carbon Dioxide" (TO_call03_2012_0135): 2013-2016 (355300€)
- CRT project "Carbon dioxide, from problem to opportunity: electrocatalytic and photocatalytic reduction of CO₂ for an eco-sustainable economy" 2015-2017 (about 35000€)
- SATURNO project "Organic waste and carbon dioxide transformed into fuels, fertilizers and chemical products; concrete application of the circular economy" funded by the Piedmont Region 2017-2021 (€116,683).
- Dompè Farmaceutici "determination of crystalline structures of molecules of pharmaceutical interest by means of computational methods" 2019-2020 (34000€).
- Dompè Farmaceutici "Crystal Structure Prediction (CSP)" (€ 60000).
- Ex Post project (31-12-2021 31-12-2023, € 58705) on Solid State Batteries

- MetCCUS project (H2020) "JRP-v01 Metrology support for carbon capture utilization and storage" (2022-2025,).
- CRF (Centro Ricerche Fiat, € 105000) for a PhD on Solid State Li ion Batteries
- HYSYTECH "developing electrochemical cell for electrochemical reduction of CO₂"€ 30000
- PRIN 2022 "CArbon Dloxide VAlorization by chemical, Photo- and Electro-chemical processes" (CADIVAPE, € 376744, with Nicola Armaroli),
- Responsible of a grant from private company (<u>www.a2a.it</u>) for electrochemical conversion of CO₂ into valuable chemical products (December 2024, about € 480000)

OTHER ELEMENTS

- Steering Committee of the Interuniversity Consortium of Reactivity and Catalysts (CIRCC) and deputy representative for the University of Turin at the Consortium CIRCC since 01-03-2011.
- Steering Committee of the Interdivisional Group of Organometallic Chemistry (GICO) of the Italian Society of Chemistry: https://www.soc.chim.it/it/gruppi/organometallica/direttivo from 15-12-2015 until 31-12-2022.
- Guest Editor of the journal Molecules: Special Issue "Catalysis for Energy Storage and CO₂ Conversion", <u>http://www.mdpi.com/journal/molecules/special issues/co2 conversion</u>
- Editorial Board Member of Catalysts: <u>https://www.mdpi.com/journal/catalysts/editors</u>
- Editorial Board Member of Computational Catalysis:
 <u>https://www.mdpi.com/journal/catalysts/sectioneditors/computational_catalysis</u>
- Nominator for the VinFuture Prize (2024): <u>https://vinfutureprize.org/vinfuture-prize-nomination/</u>
- Scientific and Local Organizer of the 44th International Conference on coordination chemistry (ICCC 2022), Rimini, 31 August – 2 September 2022 (with Proff. Roberto Gobetto, Maurizio Peruzzini, Valerio Zanotti, Giuliano Giambastiani, Andrea Rossin, Stefano Zacchini). The event, assigned on 12/09/2012 at the 40th ICCC2012 meeting in Valencia (Spain), has been postponed from 2020 to 2022 due to COVID.
- Chair (with Osamu Ishitani) of the XIII° GICO Congress of the Italian Chemical Society (CoGICO 2022), subtopic 1 at the ICCC2022, Rimini, 31 August 2 September 2022.
- Served as referee for Angew. Chem., Nature Commun., Nature Chem., ACS Cat., ACS Appl. Energy Mat., ACS Appl. Mat. Interfaces, J. Am. Chem. Soc., Inorg. Chem., Organometallics, Eur. J. Inorg. Chem., Chem. Eur. J., Electrochimica Acta, Dalton Trans., RSC Advances, J. Phys. Chem. A, Inorg. Chim. Acta, ChemElectroChem, ChemPhysChem, ChemPlusChem, J. Organomet. Chem., Molecules, Catalysts and for national and international research projects (France, Czech Republic, Romania, Norway, and Italy), and European (reviewer for COST and reviewer of 19 projects H2020, year 2020: "Secure, clean and efficient energy").