CLAUDIO GRECO

Curriculum vitae et studiorum

1. PERSONAL DATA AND EMPLOYMENT HISTORY

1.1 Name: Claudio Greco
1.2 Date of birth: 29/05/1980
1.3 Gender: M
1.4 Present position: Full Professor of Physical Chemistry at the Department of Earth and Environmental Sciences, University of Milano - Bicocca (Milan, Italy).
1.5 Previous employments:

- 2008 – 2009: Post-doc position and Alexander von Humboldt Research Fellowship in Theoretical Chemistry at the laboratory of Prof. V. Bonacic-Koutecky (Humboldt-Universität zu Berlin, Germany);
- 2009 – 2011: Post-doc position at the laboratory of Prof. P. Fantucci and Prof. L. De Gioia, University of Milano - Bicocca;
- 2011 – 2012: Junior research group leader position, Humboldt-Universität zu Berlin;
- 2012 – 2017: "Ricercatore a tempo determinato" (independent faculty researcher position with teaching duties) at the Department of Earth and Environmental Sciences of the University of Milano - Bicocca.
- 2018 – 2021: Associate Professor of Physical Chemistry at the Department of Earth and Environmental Sciences of the University of Milano - Bicocca.

2. DEGREES, ASSESSMENTS AND EVALUATIONS

2.1 Academic degrees:

- November 2004 – M.Sc. in Biotechnology (Italian 5 years degree). Degree obtained at the University of Milano - Bicocca;
- December 2007 – Ph.D. in Chemistry. Degree obtained at the University of Milano - Bicocca; scientific supervisor: Prof. L. De Gioia.

2.2 Evaluations of own scientific effort: Excellent evaluation attributed to all the scientific articles presented by C.G. for the Research Quality Assessments VQR 2011-2014 and VQR 2015-2019 (initiatives promoted by the Italian National Agency for the Evaluation of Universities and Research Institutes - ANVUR).

3. GRANTED RESEARCH PROPOSALS

3.1 Selection of grants obtained as PI:

- 2011 - 2012 – Research project entitled: "A holistic QM/MM approach for the investigation of electronic and redox properties of methane oxygenases and hydrogenases". Granting organization: "UniCat" Cluster of Excellence for Catalysis, Berlin, Germany;
- 2014 – IMERA project proposal: "The interface between biochemistry, inorganic chemistry and computing to understand biological hydrogen production and CO_2 consumption". Granting organization: Institut Méditerranéen de Recherches Avancées (IMERA), Marseille, France;
- 2020 - 2021 – Call for research proposals n. 4922 - Regione Lombardia; project title: "Design, Sviluppo e Sintesi di Radiofarmaci Innovativi". Granting organization: Regione Lombardia, Italy;

3.2 Supercomputing resources allocations obtained as PI:

- 2010 - 2011 – ISCRA B HPC CINECA Grant entitled: "Protons and electrons transfer towards [FeFe]-hydrogenases active site models: fundamental hints for H_2 evolution catalysis". Granting organization: CINECA Consortium, Bologna, Italy;

- 2014 - 2015 – LISA Prod HPC CINECA Grant entitled: "Systematic ab-initio investigation of protein-imposed influence in [NiFe]-hydrogenase fragments". Granting organization: CINECA Consortium;
- 2016 - 2018 – LISA Prod HPC CINECA Grant entitled: "Molecular simulation of water adsorption processes on particulate matter models". Granting organization: CINECA Consortium.

4. INVITED PARTICIPATION TO SCIENTIFIC CONFERENCES (SELECTION)

- Talk at the Multiscale Modeling and Simulation in Science conference (Stockholm; November 2009). Title of the contribution: "Theoretical studies on the structural and catalytic properties of [FeFe]-hydrogenases and related low weight bioinspired models";
- Talk at the II Congresso Nazionale di Chimica Teorica e Computazionale (Padua, February 2013). Title of the contribution: "DFT-based design of molecular functionality: the case of hydrogenases biomimetic models";
- Talk at the tutorial session of the Bioinorganic and Theoretical Chemistry in Relation to Energy and Environment symposium (Marseille, April 2014). Title of the contribution: "QM/MM calculations of energy profile of biological reaction mechanisms";
- Talk at the XI Molybdenum and Tungsten Enzyme Conference (Potsdam, July 2019). Title of the contribution: "The dehydrogenase and hydrogenase activities of Mo/Cu-dependent CO-dehydrogenases: a theoretical perspective".

5. GRADUATE SUMMER SCHOOLS (ORGANIZED OR LECTURED AT)

- Lecturer at the XVII School of Pure and Applied Biophysics, held in 2013 in Venice, Italy
- Co-Director of the School entitled "Computational Spectroscopy: Bridging Theory and Experiment", held in 2018 in the context of the Lake Como School of Advanced Studies (Como, Italy).

6. MAIN REVIEWER/EVALUATOR ACTIVITIES

- Reviewer for more than 25 scientific journals of chemistry indexed in WoS and SCOPUS (*e.g.* Nature Catalysis, Journal of the American Chemical Society, Chemical Science, Journal of Catalysis, Journal of Computational Chemistry);
- Research projects reviewer for: US-Israel Binational Science Foundation; Croatian Science Foundation; Czech Science Foundation; Executive Agency for Higher Education, Research, Development and Innovation Funding (Romania); CINECA Consortium (Italy);
- External evaluator/public examiner in Ph.D. Commissions at the following institutes: Technische Universität Berlin, Germany (2017); Università di Milano - Bicocca, Italy (2020).

7. MAIN ADMINISTRATIVE AND REPRESENTATIVE DUTIES

- Vice Director of the Department of Earth and Environmental Sciences, University of Milano - Bicocca (November 2019 – present);
- Vice President, Division of Theoretical and Computational Chemistry ("Divisione di Chimica Teorica e Computazionale", DCTC) of the Italian Chemical Society (February 2020 – present);
- Member of the Quality Assurance Committee of the University of Milano - Bicocca (April 2021 – present);
- Member of the Academic Senate of the University of Milano - Bicocca (October 2021 – present).

8. HONORS AND AWARDS

- Alexander von Humboldt Research Fellowship (May 2008 – April 2009);
- Special Mention, Eolo Scrocco Prize 2012 (presented by the DCTC, Italian Chemical Society);
- Carla Roetti Medal 2019 (a prize presented by the DCTC, Italian Chemical Society).

List of publications authored or co-authored by Claudio Greco

Papers published in internationally reputed periodicals, which have been subject to referees' assessment:

1) Greco C.; Sacco E.; Vanoni M.; De Gioia L. (2005) "Identification and in silico analysis of a new group of double-histone fold-containing proteins"; *Journal of Molecular Modeling* 12:76-84

2) Greco C.; Fantucci P.; De Gioia L. (2005) "In silico functional characterization of a double histone fold domain from the *Heliothis zea* virus 1"; *BMC Bioinformatics* 6 (Suppl.4):S15

3) Zampella G.; Greco C.; Fantucci P.; De Gioia L. (2006) "Proton reduction and dihydrogen oxidation on models of the $[2Fe]_H$ cluster of [Fe] hydrogenases. A density functional theory investigation"; *Inorganic Chemistry*, 45:4109-4118

4) Bertini L.; Greco C.; De Gioia L.; Fantucci P. (2006) "Time-dependent density functional theory study of $Fe_2(CO)_9$ low-lying electronic excited states"; *Journal of Physical Chemistry A*, 110:12900-12907

5) Briani F.; Del Favero M.; Capizzuto R.; Consonni C.; Zangrossi S.; Greco C.; De Gioia L.; Tortora P.; Deho G. (2007) "Genetic analysis of polynucleotide phosphorylase structure and functions"; *Biochimie*, 89:145-157

6) Schneider C.J.; Zampella G.; Greco C.; Pecoraro V.L.; De Gioia L. (2007) "Mechanistic analysis of nucleophilic substrates oxidation by functional models of Vanadium-dependent haloperoxidases: a density functional theory study"; *European Journal of Inorganic Chemistry*, 515-523

7) Greco C.; Zampella G.; Bertini L.; Bruschi M.; Fantucci P.; De Gioia L. (2007) "Insights into the mechanism of electrocatalytic hydrogen evolution mediated by $Fe_2(S_2C_3H_6)(CO)_6$: the simplest functional model of the Fe-hydrogenase active site"; *Inorganic Chemistry* 46:108-116

8) Greco C.; Bruschi M.; Fantucci P.; De Gioia L. (2007) "Influence of a large σ-donor ligand on structural and catalytic properties of di-iron compounds related to the active site of Fe-hydrogenase. A DFT investigation"; *European Journal of Inorganic Chemistry*, 1835-1843

9) Greco C.; Bruschi M.; De Gioia L.; Ryde U. (2007) "A QM/MM investigation of the activation and catalytic mechanism of Fe-only hydrogenases"; *Inorganic Chemistry*, 46:5911-5921

10) Greco C.; Bruschi M.; Heimdal J.; Fantucci P.; De Gioia L.; Ryde U. (2007) "Structural insights into the active-ready form of [FeFe]-hydrogenase and mechanistic details of its inhibition by carbon monoxide"; *Inorganic Chemistry*, 46:7256-7258

11) Bertini L.; Bruschi M.; De Gioia L.; Fantucci P.; Greco C.; Zampella G. (2007) "Quantum chemical investigations of reaction paths of metalloenzymes and biomimetic models - The hydrogenase example"; *Topics in Current Chemistry* 268:1-46

12) Bruschi M.; Greco C.; Fantucci P.; Ryde U.; De Gioia L. (2008) "A DFT investigation on structural and redox properties of a synthetic Fe_6S_6 assembly closely related to the [FeFe]-hydrogenases active site"; *Comptes Rendus Chimie*, 11:834-841

13) Bruschi M.; Greco C.; Fantucci P.; De Gioia L. (2008) "Structural and electronic properties of the [FeFe] hydrogenase H-cluster in different redox and protonation states. A DFT investigation"; *Inorganic Chemistry*, 47:6056-6071

14) Bruschi M.; Greco C.; Kaukonen M.; Fantucci P.; Ryde U.; De Gioia L. (2009) "Influence of the $[2Fe]_H$ subcluster environment on the properties of key intermediates in the catalytic cycle of [FeFe] hydrogenases. Hints for the rational design of synthetic catalysts"; *Angewandte Chemie Int. Ed.*, 48:3503-3506

15) Greco C.; Bruschi M.; Fantucci P.; De Gioia L. (2009) "Relation between coordination geometry and stereoelectronic properties in DFT models of the CO-inhibited [FeFe]-hydrogenase cofactor"; *Journal of Organometallic Chemistry*, 694:2846-2853

16) Bertini L.; Greco C.; De Gioia L.; Fantucci P. (2009) "DFT/TDDFT exploration of the potential energy surfaces of the ground state and excited states of $Fe_2(S_2C_3H_6)(CO)_6$, a simple functional model of the [FeFe] hydrogenase active site"; *The Journal of Physical Chemistry A*, 113:5657-5670

17) Joly L.; Antoine R.; Albrieux F.; Ballivian R.; Broyer M.; Chirot F.; Lemoine J.; Dugourd P.; Greco C.; Mitric R.; Bonacic-Koutecky V. (2009) "Optical and structural properties of copper-oxytocin dications in the gas phase"; *The Journal of Physical Chemistry B*, 113:11293-11300

18) Ryde U.; Greco C.; De Gioia L. (2010) "Quantum refinement of [FeFe] hydrogenase indicates a dithiomethylamine ligand"; *Journal of the American Chemical Society*, 132:4512-4513

19) Bertini L.; Greco C.; Bruschi M.; Fantucci P.; De Gioia L. (2010) "CO affinity and bonding properties of [FeFe] hydrogenase active site models. A DFT study"; *Organometallics*, 29:2013-2025

20) Greco C.*; Fantucci P.; De Gioia L.*; Suarez-Bertoa R.; Bruschi M.; Talarmin J.; Schollhammer P. (2010) "Electrocatalytic dihydrogen evolution mechanism of $[Fe_2(CO)_4(\kappa^2\text{-}Ph_2PCH_2CH_2PPh_2)(\mu\text{-}S(CH_2)_3S)]$ and related models of the [FeFe]-hydrogenase active site: a DFT investigation"; *Dalton Transactions*, 39:7320-7329

21) Bruschi M.; Greco C.; Bertini L.; Fantucci P.; Ryde U.; De Gioia L. (2010) "Functionally relevant interplay between the Fe_4S_4 cluster and CN^- ligands in the active site of [FeFe]-hydrogenases"; *Journal of the American Chemical Society*, 132:4992-4993

22) Greco C.*; Fantucci P.; Ryde U.; De Gioia L. (2010) "Fast generation of broken symmetry states in a large system including multiple iron-sulfur assemblies: investigation of QM/MM energies, clusters charges and spin populations"; *International Journal of Quantum Chemistry*, 111:3949-3960

23) Greco C.*; Bruschi M.; Fantucci P.; Ryde U.; De Gioia L. (2011) "Isocyanide in biochemistry? A theoretical investigation on the electronic effects and on the energetics of cyanide ligand protonation in [FeFe]-hydrogenases"; *Chemistry – A European Journal*, 17:1954-1965

24) Greco C.*; Silakov A.*; Bruschi M.; Ryde U.; De Gioia L.; Lubitz W. (2011) "Magnetic properties of [FeFe]-hydrogenases: a theoretical investigation based on extended QM and QM/MM models of the H-cluster and its surroundings"; *European Journal of Inorganic Chemistry*, 7:1043-1049

25) Yu L.; Greco C.; Bruschi M.; Ryde U.; De Gioia L.; Reiher M. (2011) "Targeting intermediates of [FeFe]-Hydrogenase by CO and CN vibrational signatures"; *Inorganic Chemistry*, 50:3888-3900

26) Baffert C. Bertini L.; Lautier T.; Greco C.; Sybirna K.; Ezanno P.; Etienne E.; Soucaille P.; Bertrand P.; Bottin H.; Meynial-Salles I.; De Gioia L.; Léger C. (2011) "Exogenous CO disrupts the reduced H-cluster of FeFe hydrogenase. A combined DFT and PFV study"; *Journal of the American Chemical Society*, 133:2096-2099

27) Greco C.*; De Gioia L. (2011) "A Theoretical Study on the Enhancement of Functionally Relevant Electron Transfers in Biomimetic Models of [FeFe]-Hydrogenases"; *Inorganic Chemistry*, 50:6987-6995

28) Greco C.*; Bruschi M.; Fantucci P.; Ryde U.; De Gioia L.* (2011) "Mechanistic and physiological implications of the interplay among iron-sulfur clusters in [FeFe]-hydrogenases. A QM/MM perspective"; *Journal of the American Chemical Society*, 133:18742-18749

29) Greco C.*; Bruschi M.; Fantucci P.; Ryde U.; De Gioia L.* (2011) "Probing the effects of one-electron reduction and protonation on the electronic properties of the Fe-S clusters in the active-ready form of [FeFe]-hydrogenases. A QM/MM investigation"; *ChemPhysChem*, 17:3376-3382

30) Sacco E.; Farina M.; Greco C.; Lamperti S.; Busti S.; De Gioia L.; Alberghina L.; Liberati D.; Vanoni M. (2012) "Regulation of hSos1 activity is a system-level property generated by its multi-domain structure"; *Biotechnology Advances*, 30:154-168

31) Bertini L.; Bruschi M.; Romaniello M.; Zampella G.; Tiberti M.; Barbieri V.; Greco C.; La Mendola D.; Bonomo R.P.; Fantucci P.; De Gioia L. (2012) "Copper coordination to the putative cell binding site of angiogenin. A DFT investigation"; *Theoretical Chemistry Accounts*, 131, article n. 1186

32) Heims F.; Mereacre V.; Ciancetta A.; Mebs S.; Powell A.K.; Greco C.; Ray K. (2012) "Synthesis and spectroscopic characterisation of a heterodinuclear iron(III)-copper(II) complex based on an asymmetric dinucleating ligand system"; *European Journal of Inorganic Chemistry*, 4565-4569

33) Goetze J.; Greco C.; Mitric R.; Bonacic-Koutecky V. Saalfrank P. (2012) "BLUF hydrogen network dynamics and UV/vis spectra: a combined molecular dynamics and quantum chemical study"; *Journal of Computational Chemistry*, 33:2233-2242

34) Kundu S.; Miceli E.; Farquhar E.; Pfaff F.F.; Kuhlmann U.; Hildebrandt P.; Braun B.; Greco C.; Ray K. (2012) "Lewis acid trapping of an elusive copper-tosylnitrene intermediate using scandium triflate"; *Journal of the American Chemical Society*, 134: 14710-14713

35) Greco C.* (2013) "H_2 binding and splitting on a new-generation [FeFe]-hydrogenase model featuring a redox-active decamethylferrocenyl phosphine ligand: A theoretical investigation"; *Inorganic Chemistry*, 52:1901-1908

36) Miyake T.; Bruschi M.; Cosentino U.; Baffert C.; Fourmond V.; Léger C.; Moro G.; De Gioia L.;* Greco C.* (2013) "Does the environment around the H-cluster allow coordination of the pendant amine to the catalytic iron center in [FeFe] hydrogenases? Answers from theory"; *Journal of Biological Inorganic Chemistry*, 18:693-700

37) Greco C.* (2013) "Towards [NiFe]-hydrogenase biomimetic models that couple H_2 binding with functionally relevant intramolecular electron transfers: a quantum chemical study"; *Dalton Transactions*, 42:13845-13854.

38) Munery S.; Capon J.-F., De Gioia L.; Elleouet C.; Greco C.; Petillon F.Y.; Schollhammer P.; Talarmin J.; Zampella G. (2013) "Novel FeI-FeI complex featuring a rotated conformation related to $[2Fe]_H$ subsite of the [Fe-Fe]H_2ase"; *Chemistry – A European Journal*, 19:15458-15461

39) Haack P.; Kaergel A.; Greco C.; Dokic J.; Braun B.; Pfaff F.F.; Mebs S.; Ray K.; Limberg C. (2013) "Access to a Cu^{II}-O-Cu^{II} Motif: Spectroscopic Properties, Solution Structure, and Reactivity"; *Journal of the American Chemical Society*, 135:16148-16160

40) Carzaniga T.; Mazzantini E.; Nardini M.; Regonesi M.E.; Greco C.; Briani F.; De Gioia L.; Tortora P.; Deho G. (2014) "A conserved loop in polynucleotide phosphorylase (PNPase) essential for both RNA and ADP/phosphate binding"; *Biochimie*, 97:49-59

41) Sicolo S.; Bruschi M.; Bertini L.; Zampella G.; Filippi F.; Arrigoni F.; De Gioia L.*; Greco C.* (2014) "Towards biomimetic models of the reduced [FeFe]-hydrogenase that preserve the key structural features of the enzyme active site; a DFT investigation"; *International Journal of Hydrogen Energy*, 39:18565-18573

42) Fourmond V.*; Greco C.; Sybirna K.; Baffert C.; Wang P.-H.; Ezanno P.; Montefiori M.; Bruschi M.; Meynial-Salles, I.; Soucaille, P.; Blumberger J.; Bottin H.; De Gioia L.; Léger C. (2014) "The oxidative inactivation of FeFe hydrogenase reveals the flexibility of the H-cluster"; *Nature Chemistry*, 6:336-342

43) Heims F.; Pfaff F.F.; Abram S.-L.; Farquhar E.; Bruschi M.; Greco C.; Ray K. (2014) "Redox non-innocence of a N-heterocyclic nitrenium cation bound to a nickel-cyclam core"; *Journal of the American Chemical Society*, 136:582-585

44) Greco C.; Moro G.; Bertini L.; Biczysko M.; Barone V.; Cosentino U. (2014) "Computational investigation on the spectroscopic properties of thiophene based europium β-diketonate complexes"; *Journal of Chemical Theory and Computation*, 10:767-777

45) Bertini L.; Greco C.; Fantucci P.; De Gioia L. (2014) "TDDFT modelling of the CO-photolysis of $Fe_2(S_2C_3H_6)(CO)_6$, a model of the [FeFe]-Hydrogenase catalytic site"; *International Journal of Quantum Chemistry*, 114:851-861

46) Greco C., Fourmond V.; Baffert C.; Wang P.-H.; Dementin S.; Bertrand P.; Bruschi M.; Blumberger J.; De Gioia L.; Léger C. (2014) "Combining experimental and theoretical methods to learn about the reactivity of gas-processing metalloenzymes"; *Energy & Environmental Science*, 7:3543-3573

47) Mulder D.W.; Ratzloff M.W.; Bruschi M.; Greco C.; Koonce E.; Peters J.W.; King P.W. (2014) "Investigations on the role of proton-coupled electron transfer in hydrogen activation by [FeFe]-hydrogenase"; *Journal of the American Chemical Society*, 136:15394-15402

48) Beaume L.; Clémancey M.; Blondin G.*; Greco C.*; Pétillon F.Y.; Schollhammer P.*; Talarmin J.* (2014) "A new systematic route to mixed-valence triiron clusters derived from dinuclear models of the active site of [Fe-Fe] hydrogenases"; *Organometallics*, 33:6290-6293

49) Greco C.*; Ciancetta A.; Bruschi M.; Kulesza A.; Moro G.; Cosentino U.* (2015) "Influence of key amino acid mutation on active site structure and on folding in Acetyl-CoA synthase: a theoretical perspective"; *Chemical Communications*, 51:8551-8554

50) Butera V.; Russo N.; Cosentino U.; Greco C.; Moro G.; Pitea D.; Sicilia E (2016) "Computational insight on CO_2 fixation to produce styrene carbonate assisted by a single centre Al(III) catalyst and quaternary ammonium salts"; *ChemCatChem*, 8:1167-1175

51) Sensi M.; Baffert C.; Greco C.; Caserta G.; Gauquelin C.; Saujet L.; Fontecave M.; Roy S.; Artero V.; Soucaille P.; Meynial-Salles I.; Bottin H.; De Gioia L.; Fourmond V.; Léger C.; Bertini L. (2016) "Reactivity of the excited states of the H-cluster of FeFe hydrogenases"; *Journal of the American Chemical Society*, 138:13612-13618

52) Breglia R.; Ruiz Rodriguez M.A.; Vitriolo A.; Gonzales Laredo R.F.; De Gioia L.; Greco C.; Bruschi M. (2017) "Theoretical insights into [NiFe]-hydrogenases oxidation resulting in a slowly reactivating inactive state"; *Journal of Biological Inorganic Chemistry*, 22:137-151

53) Breglia R.; Bruschi M.; Cosentino U.; De Gioia L.; Greco C.*; Miyake T.; Moro G. (2017) "A theoretical study on the reactivity of the Mo/Cu containing carbon monoxide dehydrogenase with dihydrogen"; *Protein Engineering, Design, and Selection*, 30:169-174

54) D'Arienzo M.; Gamba L.; Morazzoni F.; Cosentino U.; Greco C.; Lasagni M.; Pitea D.; Moro G.; Cepek C.; Butera V.; Sicilia E.; Russo N.; Munoz-Garcia A.B.; Pavone M. (2017) "Experimental and theoretical investigation on the catalytic generation of environmentally persistent free radicals from benzene"; *Journal of Physical Chemistry C*, 121:9381-9393

55) Cosentino U.*; Greco C.*; Pitea D.; Binetti S.; Le Donne A.; Moro G.; Baiardi A. (2017) "Theoretical and experimental investigation of UV-vis absorption spectrum in a Eu(3+) based complex for luminescent down shifting applications"; *Theoretical Chemistry Accounts*, 136:117

56) Monte-Pérez I.; Kundu S.; Chandra A.; Craigo K.; Chernev P.; Kuhlmann U.; Dau H.; Hildebrandt P.; Greco C.; Van Stappen C.; Lehnert N.; Ray K. (2017) "Temperature dependence of the catalytic two- versus four-electron reduction of dioxygen by a hexanuclear cobalt complex"; *Journal of the American Chemical Society*, 139:15033-15042

57) Rovaletti A.; Greco C.* (2018) "Organophosphorous ligands in hydrogenase-inspired iron based catalysts: a DFT study on the energetics of metal protonation as a function of P-atom substitution"; *Journal of Physical Organic Chemistry*, 31:e3748

58) Breglia R.; Greco C.; Fantucci P.; De Gioia L.; Bruschi M. (2018) "Theoretical investigation of aerobic and anaerobic oxidative inactivation of the [NiFe]-hydrogenase active site"; *Physical Chemistry Chemical Physics*, 20:1693-1706

59) Del Barrio M.; Sensi M.; Fradale L.; Bruschi M.; Greco C.; de Gioia L.; Bertini L.; Fourmond V.; Léger C. (2018) "Interaction of the H-cluster of FeFe hydrogenase with halides"; *Journal of the American Chemical Society*, 140:5485-5492

60) Giorgetti S.; Greco C.; Tortora P.; Aprile F.A. (2018) "Targeting amyloid aggregation: an overview of strategies and mechanisms"; *International Journal of Molecular Sciences*, 19:e2677

61) Rovaletti, A.; Bruschi M.; Moro G.; Cosentino U. Greco C.* (2019) "The challenging in silico description of CO-dehydrogenase activity in Mo-Cu carbon monoxide dehydrogenase"; *Frontiers in Chemistry*, 6:630

62) Breglia R.; Greco C.; Fantucci P.; De Gioia L.; Bruschi M. (2019) "Reactivation of the ready and unready oxidized states of [NiFe]-hydrogenases: mechanistic insights from DFT calculations"; *Inorganic Chemistry*, 58:279-293

63) Arrigoni F.; Bertini L.; Bruschi M.; Greco C.; De Gioia L.; Zampella G. (2019) "H_2 activation in [FeFe]-Hydrogenase cofactor versus diiron dithiolate models: factors underlying the catalytic success of nature and implications for an improved biomimicry"; *Chemistry - A European Journal*, 25:1227-1241

64) Greco C.; Cosentino U.; Pitea D.; Moro G.; Santangelo S.; Patanè S.; D'Arienzo M.; Fiore M.; Morazzoni F.; Ruffo R. (2019) "Role of the carbon defects in the catalytic oxygen reduction by graphite nanoparticles: a spectromagnetic, electrochemical and computational integrated approach"; *Physical Chemistry Chemical Physics*, 21:6021-6032

65) Rovaletti A.; Bruschi M.; Moro G.; Cosentino U.; Ryde U.*; Greco C.* (2019) "A thiocarbonate sink on the enzymatic energy landscape of aerobic CO oxidation? Answers from DFT and QM/MM models of Mo-Cu CO-dehydrogenases"; *Journal of Catalysis*, 372:201-205

66) Rovaletti A.; Bruschi M.; Moro G.; Cosentino U.; Greco C.*; Ryde U.* (2019) "Theoretical Insights into the Aerobic Hydrogenase Activity of Molybdenum-Copper CO Dehydrogenase"; *Inorganics*, 7:135

67) Shimamura T.; Maeno Y.; Kubo K.; Kume S.; Greco C.; Mizuta T. (2019) "Protonation and Electrochemical Properties of Bisphosphide Diiron Hexacarbonyl Complex Bearing Amino Groups on the Phosphide Bridge"; *Dalton Transactions*, 48:16595-16603

68) Caserta G.; Lorent C.; Ciaccafava A.; Keck M.; Breglia R.; Greco C.; Limberg C.; Hildebrandt P.; Cramer S.P.; Zebger I.; Lenz O. (2020) "The large subunit of the regulatory [NiFe]-hydrogenase from *Ralstonia eutropha* – A minimal hydrogenase?"; *Chemical Science*, 11:5453-5465

69) Sala D.; Cosentino U.; Ranaudo A.; Greco C.*; Moro G.* (2020) "Dynamical Behavior and Conformational Selection Mechanism of the Intrinsically Disordered Sic1 Kinase-Inhibitor Domain"; *Life*, 10:110

70) Arrigoni F.; Bertini L.; Breglia R.; Greco C.; De Gioia L.; Zampella G. (2020) "Catalytic H_2 Evolution/Oxidation in [FeFe]-Hydrogenase Biomimetics: Account from DFT on the Interplay of Related Issues and Proposed Solutions"; *New Journal of Chemistry*, 44:17596-17615

71) Arrigoni F.; Rizza F.; Vertemara J.; Breglia R.; Greco C.; Bertini L.; Zampella G.; De Gioia L. (2020) "Rational design of $Fe_2(\mu\text{-}PR_2)_2(L)_6$ coordination compounds featuring tailored potential inversion"; *ChemPhysChem*, 21:2279-2292.

72) Breglia R.; Arrigoni F.; Sensi M.; Greco C.*; Fantucci P.; De Gioia L.*; Bruschi M. (2021) "First-principles calculations on Ni,Fe-containing carbon monoxide dehydrogenases reveal key stereoelectronic features for binding and release of CO_2 to/from the C-cluster"; *Inorganic Chemistry*, 60:387402.

73) Hobballah A.; Arrigoni F.*; Elleouet C.*; Greco C.*; Laurans M.; Ptillon F.Y.; Schollhammer P.* (2021) "Triiron clusters derived from dinuclear complexes related to the active site of [Fe-Fe] hydrogenases: Steric effect of the dithiolate bridge on redox properties, a DFT analysis"; *Inorganic Chemistry Frontiers*, 8:3659-3674.

74) Arrigoni F.; Zampella G.; De Gioia L.; Greco C.*; Bertini L.* (2021) "The Photochemistry of $Fe_2(S_2C_3H_6)(CO)_6(\mu\text{-}CO)$ and its Oxidized Form, Two Simple [FeFe]-Hydrogenase CO-Inhibited Models. A DFT and TDDFT Investigation"; *Inorganics*, 9:16

75) Rovaletti A.; Greco C.*; Ryde U.* (2021) "QM/MM study of the binding of H_2 to MoCu CO dehydrogenase: development and applications of improved H_2 van der Waals parameters"; *Journal of Molecular Modeling*, 27:68.

76) Arrigoni F.; Rovaletti R.; Bertini L.; Breglia R.; De Gioia L.; Greco C.; Vertemara J.; Zampella G.; Fantucci P. (2022) "Investigations of the electronic-molecular structure of bio-inorganic systems using modern methods of quantum chemistry"; *Inorganica Chimica Acta*, 532:120728.

77) Rovaletti A.; Moro G.; Cosentino U.; Ryde U.*; Greco C.* (2022) "Can water act as a nucleophile in CO oxidation catalysed by Mo/Cu CO-dehydrogenase? Answers from theory"; *ChemPhysChem*, 23:e202200053.

78) Vaghi L.; Rizzo F.; Pedrini J.; Mauri A.; Meinardi F.; Cosentino U.; Greco C.; Monguzzi A.; Papagni A. (2022) "Bypassing the statistical limit of singlet generation in sensitized upconversion using fluorinated conjugated systems"; *Photochemical & Photobiological Sciences*, 21:913-921.

79) Ritacca A.G.; Rovaletti A.*; Moro G.; Cosentino U.; Ryde U.*; Sicilia E.; Greco C.* (2022) "Unraveling the reaction mechanism of Mo/Cu CO dehydrogenase using QM/MM calculations"; *ACS Catalysis*, 12:7336-7343.

80) Decavoli C.; Boldrini C. L.; Faroldi F.; Baldini L.; Sansone F.; Ranaudo A.; Greco C.; Cosentino U.: Moro G.; Manfredi N.; Abbotto A. (2022) "Calix[4]arene-based sensitizers for host-guest supramolecular dyads for solar energy conversion in photoelectrochemical cells"; *European Journal of Organic Chemistry*, in press.

Other publications (refereed book chapters, PhD thesis, preprints currently under review):

81) Greco C. "A DFT and QM/MM investigation on models related to the [FeFe]-hydrogenase active site"; (2007) PhD Thesis, Univ. Milano - Bicocca, Milan, Italy

82) Bruschi M.; Zampella G.; Greco C.; Bertini L.; Fantucci P.; De Gioia L. (2009) "Hydrogenases: theoretical investigations towards bioinspired H_2 production and activation"; in: 'Computational Inorganic and Bioinorganic Chemistry'; Solomon, E. I.; King, R. B.; Scott, R. A., Eds., *The Encyclopedia of Inorganic Chemistry*, published by John Wiley & Sons, Chichester, UK

83) Bertini L.; Bruschi M.; Cosentino U.; Greco C.; Moro G.; Zampella G.; De Gioia L. (2014) "Quantum mechanical methods for the investigation of metalloproteins and related bioinorganic compounds"; book chapter in 'Handbook on Metalloproteins'; Walker, J.M., Fontecilla-Camps J., Eds., *Methods in Molecular Biology*, published by Springer Science+Business Media

84) Greco C.; De Gioia L. (2014) "DFT investigation of models related to the active site of hydrogenases"; book chapter in 'Bioinspired Catalysis: Metal-Sulfur Complexes'. Editor: Schollhammer, P.; published by John Wiley & Sons

85) Breglia R.; De Gioia L.; Greco C.; Bruschi M. (2018) "Theory related to [FeFe]- and [NiFe]-hydrogenases: stereoelectronic properties, H-cluster oxidation, and mechanisms for increasing oxygen tolerance"; book chapter in 'Microalgal Hydrogen Production: Achievements and Perspectives'. Editors: G. Torzillo and M. Seibert. Publisher: Royal Society of Chemistry.

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