ALLEGATO B

**DICHIARAZIONI SOSTITUTIVE DI CERTIFICAZIONI**
(art. 46 D.P.R. n. 445/2000)
**DICHIARAZIONI SOSTITUTIVE DELL'ATTO DI NOTORIETÀ**
(art. 47 D.P.R. n. 445/2000)

Il Sottoscritto
**COGNOME** Capone
**NOME** Matteo

egolamentari in
ge 12 novembre
i e dichiarazioni
falsità negli atti
dichiara sotto la

preciso delle informazioni sulla
risponde a verità

## Current Position

Sep.2023– Present **Student Fellowship**, UNIVERSITÀ DELL'AQUILA, Department of Physical and Chemical Science.
Study of the catalytic activity of enzymes by means of molecular dynamics simulations and quantum mechanical calculations

## Professional Experience and Academic Titles

Sep.2022– Aug.2023 **Post-Doc Researcher**, UNIVERSITÀ DELL'AQUILA, Department of Physical and Chemical Science.
Systematic parameterization of classical force fields for drug-like molecules from quantum chemical data. Supervisors: Prof. Isabella Daidone, PhD Giacomo Prampolini (ICCOM-CNR Pisa)

Mar.2020– Jun.2023 **Tutor in Chemistry courses**, UNIVERSITÀ DELL'AQUILA, Department of Industrial Engineering, Information and Economy.

2020–2021 **Cultore della Materia in Chemistry**, UNIVERSITÀ DELL'AQUILA, Department of Industrial Engineering, Information and Economy.

Jun.2020– Jun.2022 **Post-Doc Researcher**, UNIVERSITÀ DELL'AQUILA, Department of Physical and Chemical Science.
Proton transfer processes in protein environment. Supervisor: Prof. Isabella Daidone

Dec.2019– May.2020 **Student Fellowship**, UNIVERSITÀ DELL'AQUILA, Department of Physical and Chemical Science.
Molecular dynamics simulations of enzymes with oxidative and hydrolytic activity. Supervisor: Prof. Leonardo Guidoni

Nov.2016– Oct.2019 **PhD in Mathematics and Models**, UNIVERSITÀ DELL'AQUILA, Department of Information Engineering, Computer Science and Mathematics.
Defense date: 6/5/2020, Protocol: 12124/37, Thesis title: Multiscale molecular modeling of photosynthetic water oxidation mechanism. Supervisor: Prof. Leonardo Guidoni

Mar.2016– Sep.2016 **Student Fellowship**, UNIVERSITÀ DELL'AQUILA, Department of Physical and Chemical Science.
Simulation of Vibrational properties of Photosystem-II using Molecular Dynamics based methods.

L'AQUILA 21/12/2023

Oct.2013–Dec.2015 **Master Degree in Chemical Sciences**, SAPIENZA UNIVERSITÀ DI ROMA, Curricula: Biological Systems Chemistry, *110/110 cum Laude*.
Defence date: 16/12/2015 Protocol: 12124/37, Thesis Title: Studio del centro di reazione del Fotosistema II con metodi di chimica quantistica (*Photosystem II reaction centre study by means of quantum chemistry methods*), Supervisors: Prof. Leonardo Guidoni and Prof. Ruggero Caminiti

Oct.2010–Dec.2013 **Bachelor Degree in Chemical Sciences**, SAPIENZA UNIVERSITÀ DI ROMA, *98/110*.
Defence date: 11/12/2013, Protocol: 11108/51, Thesis Title: Sintesi di building blocks per la preparazione di fosfodiesterasi artificiali (*Synthesis of building blocks for the preparation of artificial phosphodiestherases*), Supervisor: Dr. Riccardo Salvio

## Post Graduate Courses

**Paris International School on Advanced Computational Material Science 2019**, *Sorbonne University, Paris, France.*

**Summer School on Electronic Structure and Spectroscopy of Transition Metal Complexes 2017**, *MPI-CEC, Gelsenkirchen, Germany.*

## Oral Contribution to Conferences

Sep. 2023 VIII Congress of the Italian Chemical Society - Theoretical Computational Chemistry Division, Scuola Normale Superiore, Pisa

Aug. 2023 European Chemistry Society - Computational Chemistry Congress - Thessaloniki, Greece.

Jul. 2023 CT4OPTO Workshop, Principles of light-induced charge transfer for optogenetics, Università di Modena

Sep. 2022 VII Congress of the Italian Chemical Society - Theoretical Computational Chemistry Division, Università di Modena

Feb. 2022 Winter Modeling Workshop. Scuola Superiore Meridionale, Napoli

Apr. 2022 Workshop of Italian Chemical Society - Theoretical Computational Chemistry Division, Università di Firenze

Sep. 2021 XXVII National Congress of Italian Chemical Society

July 2019 XLVII Congress of Italian Chemical Society - Chemical Physics Division, Sapienza Università di Roma.

Oct. 2018 BUUR (Berlin Umea Uppsala Rome) Meeting, Workshop on photosynthesis research, Freie Universitat Berlin, Germany.

June 2018 European Congress on Photosynthesis Research, University of Uppsala, Sweden

## Other Scientific Activities

2020–Present Scientific Popularizer and Communicator as "Il Chimico Sulla Tavola" on Web, Social and live.

Live events: CICAP Fest2023 Padova; Food&Science Festival 2023 Mantova; AISPEC @ In-Vitality 2021 (Chairing) ; SCI Abruzzo "Giochi della Chimica 2021" Award Ceremony; European Night of Reserchers - Street Science (Organization and Event hosting).

On-line Orientation for high schoolers: Federchimica-PLS Orientagiovani 2022&2023 (Chairing)

2020 Finalist of the popularization talent show "FameLab Italia"

2017 Organization of BUUR (Berlin Umea Uppsala Rome) Meeting, Workshop on photosynthesis research, Sapienza Università di Roma, Italy

## Awards and Honors

2023 Awarded with the "Eolo Scrocco" prize by the Italian Chemical Society - Division of Theoretical and Computational Chemistry (DCTC) for a young and talented reseacher



L'AQUILA 27/12/2023

2023 Awarded with best oral presentation in "Biological Systems" field at EuChemS-CompChem Congress in Thessaloniki, Greece.

## Other Skills

**Software** ORCA, CP2K, GAUSSIAN, GROMACS, VMD, PYMOL, GNUPLOT, GIMP IMAGE EDITOR, OFFICE SUITE PROGRAMS

**Programming languages** PHYTHON(GOOD), FORTRAN (BASIC), BASH(GOOD), LATEX(GOOD)

**Spoken Languages** Italian: Native; English: C1; Spanish: Basic

**Soft Skills** Curious, motivated and optimistic. Fast learner. Reliable. Strong innovating and lateral thinking skills. Enjoys working in a multicultural environment. Excellent communication and networking capabilities.

**Consapevole che, ai sensi dell'art.76 del DPR 445/2000, le dichiarazioni mendaci, la falsità negli atti e l'uso di atti falsi sono punite ai sensi del Codice penale e delle leggi speciali vigenti in materia, dichiara sotto la propria responsabilità che quanto dichiarato nel curriculum vitae et studiorum comprensivo delle informazioni sulla produzione scientifica corrisponde a verità.**

L'AQUILA 21/12/2023

## List of Publications

2023 *M Capone, G Dell'Orletta, B T Nicholls, G D Scholes, T K Hyster, M Aschi, I Daidone.* Evidence of a Distinctive Enantioselective Binding Mode for the Photoinduced Radical Cyclization of $\alpha$-Chloroamides in Ene-Reductases, **ACS Catal. 13, 15310–15321**

2023 *A Vetrano, I Daidone, N Spreti, M Capone.* A combined experimental and computational approach for the rationalization of the catalytic activity of lipase B from Candida antarctica in water-organic solvent mixtures, **J. Chem. Technol. Biotechnol. 98(10), 2429-2436.**

2023 *P Greife, M Schonborn, M Capone, R Assuncao, D Narzi, L Guidoni, H Dau.* The electron-proton bottleneck of photosynthetic oxygen evolution, **Nature 617, 623–628.**

2023 *M Capone, A Sirohiwal, M Aschi, D A Pantazis, I Daidone.* Alternative Fast and Slow Primary Charge-Separation Pathways in Photosystem II, **Angew. Chem. Int. Ed. 135 (16), e202216276**

2023 *M Frezzini, A Scortica, M Capone, D Narzi, M Benedetti, F Angelucci, B Mattei, L Guidoni.* Molecular dynamics simulations and kinetic measurements provide insights into the structural requirements of substrate size-dependent specificity of oligogalacturonide oxidase 1 (OGOX1), **Plant Phys. Biochem., 194, 315-325.**

2022 *M Capone, L Zanetti-Polzi, I Leonzi, N Spreti, I Daidone.* Evidence for a high pKa of an aspartic acid residue in the active site of CALB by a fully atomistic multiscale approach, **J. Biomol. Struct. Dyn., 1-8**

2021 *A Scortica, M Capone, D Narzi, M Frezzini, V Scafati, M Giovannoni, F Angelucci, L Guidoni, B Mattei, M Benedetti,* A molecular dynamics-guided mutagenesis identifies two aspartic acid residues involved in the pH-dependent activity of OG-OXIDASE 1, **Plant Phys. Biochem. 169, 171-182**

2021 *M Capone, D Narzi, L Guidoni.* Mechanism of Oxygen Evolution and Mn4CaO5 Cluster Restoration in the Natural Water-Oxidizing Catalyst, **Biochemistry-us 2021, 60, 30, 2341–2348**

2020 *S Nakamura, M Capone, G Mattioli, L Guidoni,* Early-stage formation of (hydr) oxo bridges in transition-metal catalysts for photosynthetic processes, **Catal. Sci. Technol. 11 (5), 1801-1813**

2020 *M Capone, L Guidoni, D Narzi.* Structural and dynamical characterization of the S4 state of the Kok-Joliot's cycle by means of QM/MM Molecular Dynamics Simulations, **Chem. Phys. Lett. 742, 137111**

2020 *S Nakamura, M Capone, D Narzi, L Guidoni.* Pivotal role of the redox-active tyrosine in driving the water splitting catalyzed by photosystem II, **Phys. Chem. Chem. Phys. 22 (1), 273-285**

2019 *A Tichengulova, M Capone, F Pitari, L Guidoni.* Molecular Vibrations of an Oxygen-Evolving Complex and Its Synthetic Mimic, **Chem-Eur. J. 25 (58), 13385-13395**

2019 *M Capone, D Narzi, A Tychengulova, L Guidoni.* On the comparison between differential vibrational spectroscopy spectra and theoretical data in the carboxyl region of photosystem II, **Physiol. Plantarum 10.1111/ppl.12949**

2018 *D Narzi, M Capone, D Bovi, L Guidoni.* Evolution from S3 to S4 States of the Oxygen,ÂêEvolving Complex in PhotosystemII Monitored by Quantum Mechanics/Molecular Mechanics (QM/MM) Dynamics, **Chem-Eur. J. 24 (42), 10820–10828**

2016 *D Bovi, M Capone, D Narzi, L Guidoni,* Vibrational fingerprints of the Mn4CaO5 cluster in photosystem II by mixed quantum-classical molecular dynamics, **BBA-Bioenergetics 1857 (10), 1669-1677**

2016 M Capone, D Narzi, D Bovi, L Guidoni, Mechanism of Water Delivery to the Active Site of Photosystem II along the S2 to S3 Transition, **J. Phys. Chem. Lett. 7 (3), 592–596**

L'AQUILA 21/12/2022

2015 *M Capone, D Bovi, D Narzi, L Guidoni*, Reorganization of Substrate Waters between the Closed and Open Cubane Conformers during the S2 to S3 Transition in the Oxygen Evolving Complex, **Biochemistry-us 54 (42), 6439-6442**

Consapevole che, ai sensi dell'art.76 del DPR 445/2000, le dichiarazioni mendaci, la falsità negli atti e l'uso di atti falsi sono punite ai sensi del Codice penale e delle leggi speciali vigenti in materia, dichiara sotto la propria responsabilità che quanto dichiarato nel curriculum vitae et studiorum comprensivo delle informazioni sulla produzione scientifica corrisponde a verità.

L'AQUILA 27/12/2023