# EUROPEAN CURRICULUM VITAE FORMAT

## PERSONAL INFORMATION


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| Name | **SILVIA CARLOTTO** |
| Address | VIA TRASEA 4, 35131, PADOVA |
| Telephone | +39 049 827 5193 |
| E-mail | silvia.carlotto@unipd.it |
| Nationality | Italian |
| Date of birth | 1ST FEBRUARY 1980 |
| Place of birth | ARZIGNANO (VI), ITALY |
| Gender | FEMALE |


## WORK AND RESEARCH EXPERIENCE

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|---|---|
| • Dates (from – to) | **NOV 2018** |
| • Name and address of employer | Univesitat de Valencia, Spain |
| • Type of business or sector | Departamento de Química Fisica (prof. I. Tuñón) |
| • Occupation or position held | Visiting Researcher / Visiting Teacher |
| • Dates (from – to) | **JUN 2018 – AUG 2018** |
| • Name and address of employer | University of Tokyo, Japan |
| • Type of business or sector | Institute of Industrial Science (prof. Y. Umeno) |
| • Occupation or position held | Visiting Researcher |
| • Dates (from – to) | **JUN 2018** |
| • Name and address of employer | Technische Universiteit Eindhoven, The Netherlands |
| • Type of business or sector | Department of Chemical Engineering and Chemistry (prof. E. Hensen) |
| • Occupation or position held | Visiting Scientist / Visiting Lecture / Visiting Teacher |
| • Dates (from – to) | **GEN 2018 – MAY 2018** |
| • Name and address of employer | University of Geneva, Switzerland |
| • Type of business or sector | Department of Organic Chemistry (prof. A.I. Poblador-Bahamonde) |
| • Occupation or position held | Visiting Researcher |
| • Dates (from – to) | **MAR 2017 – FEB 2020** |
| • Name and address of employer | University of Padua, Padua, Italy |
| • Type of business or sector | Department of Chemical Sciences |
| • Occupation or position held | Researcher (RTDA) |
| • Dates (from – to) | **MAY 2016 - JUN 2016** |
| • Name and address of employer | University of Padua, Padua, Italy |

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| • Type of business or sector | Department of Chemical Sciences |
| • Occupation or position held | Post-Doc |
| • Main activities and responsibilities | Project title: "Studio di Superfici: proprietà Elettroniche, magnetiche, Reattività e Ordine a Lungo raggio per lo sviluppo di una conoscenza CompuChimica" |
| • Dates (from – to) | **DEC 2015 - APR 2016** |
| • Name and address of employer | University of Padua, Padua, Italy |
| • Type of business or sector | Department of Chemical Sciences |
| • Occupation or position held | Post-Doc |
| • Main activities and responsibilities | Project title: "Studio di Superfici: proprietà Elettroniche, magnetiche, Reattività e Ordine a Lungo raggio per lo sviluppo di una conoscenza CompuChimica" |
| • Dates (from – to) | **NOV 2014 - OCT 2015** |
| • Name and address of employer | University of Padua, Padua, Italy |
| • Type of business or sector | Department of Chemical Sciences |
| • Occupation or position held | Post-Doc |
| • Main activities and responsibilities | Project title: "Studio di Superfici: proprietà Elettroniche, magnetiche, Reattività e Ordine a Lungo raggio per lo sviluppo di una conoscenza CompuChimica" |
| • Dates (from – to) | **NOV 2012 - OCT 2014** |
| • Name and address of employer | University of Padua, Padua, Italy |
| • Type of business or sector | Department of Chemical Sciences |
| • Occupation or position held | Post-Doc |
| • Main activities and responsibilities | Project title: "Sviluppo di catalizzatori economicamente efficienti di prossima generazione" |
| • Dates (from – to) | **NOV 2011 - OCT 2012** |
| • Name and address of employer | University of Padua, Padua, Italy |
| • Type of business or sector | Department of Chemical Sciences |
| • Occupation or position held | Post-Doc |
| • Main activities and responsibilities | Project title: "In silico optimization of organic photovoltaic devices" |
| • Dates (from – to) | **APR 2011 - OCT 2011** |
| • Name and address of employer | University of Padua, Padua, Italy |
| • Type of business or sector | Department of Chemical Sciences |
| • Occupation or position held | Post-Doc |
| • Main activities and responsibilities | Project title: "Approcci multiscala alle dinamiche molecolari in soluzione" |
| • Dates (from – to) | **MAR 2009 - MAR 2011** |
| • Name and address of employer | University of Padua, Padua, Italy |
| • Type of business or sector | Department of Chemical Sciences |
| • Occupation or position held | Post-Doc |
| • Main activities and responsibilities | Project title: "Sviluppo di metodi computazionali per la descrizione di dispositivi microfluidici" |
| • Dates (from – to) | **MAR 2008 - FEB 2009** |
| • Name and address of employer | University of Padua, Padua, Italy |
| • Type of business or sector | Department of Chemical Sciences |
| • Occupation or position held | Post-Doc |
| • Main activities and responsibilities | Project title: "Sviluppo di metodi e codici di calcolo per la simulazione della risposta ottica non-lineare di cromofori multipolari in soluzione o in fase condensata" |
| • Dates (from – to) | **GEN 2008 - FEB 2008** |
| • Name and address of employer | University of Padua, Padua, Italy |
| • Type of business or sector | Department of Chemical Sciences |
| • Main activities and responsibilities | Project title: "Metodi computazionali per lo studio e le proprietà strutturali e dinamiche di nanoparticelle in sospensioni colloidali" |

## EDUCATION AND TRAINING

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| • Dates (from – to) | September 16-20, 2013 |
| • Name and type of organisation providing education and training | Imperial College, London, UK |
| • Principal subjects/occupational skills covered | International school of *Ab-Initio* Modelling in Solid State Chemistry |

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| • Dates (from – to) | 2011 |
| • Name and type of organisation providing education and training | University of Padua, Padua, Italy |
| • Principal subjects/occupational skills covered | Thesis title: "L'ascesa al Principio e la discesa: Platone e Plotino a confronto"<br>Advisor: Prof. Cristina Rossitto |
| • Title of qualification awarded | Laurea magistrale in Philosophical Sciences (specialization in ancient philosophy), grade 110/110 cum Laude |

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| • Dates (from – to) | 2008 |
| • Name and type of organisation providing education and training | University of Padua, Padua, Italy |
| • Principal subjects/occupational skills covered | Thesis title: "Il mito di Er nel libro X della *Repubblica* di Platone "<br>Advisor: Prof. Cristina Rossitto |
| • Title of qualification awarded | Laurea triennale in Philosophy (specialization in ancient philosophy), grade 110/110 cum Laude |

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|---|---|
| • Dates (from – to) | 2005-2007 |
| • Name and type of organisation providing education and training | University of Padua, Padua, Italy |
| • Principal subjects/occupational skills covered | Thesis title: "Modeling of dynamic solvation effects"<br>Advisor: Prof. Antonino Polimeno |
| • Title of qualification awarded | Ph. D. in Molecular Science (specialization Chemical Sciences) |

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| • Dates (from – to) | July 1-5, 2007 |
| • Name and type of organisation providing education and training | Tarragona, Spain |
| • Principal subjects/occupational skills covered | Electron-Nuclear Spin interaction school |

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| • Dates (from – to) | July 31 - August 11, 2006 |
| • Name and type of organisation providing education and training | University of Urbana-Champaign, Illinois, USA |
| • Principal subjects/occupational skills covered | Summer School on Computational Material Science: Ab-Initio Molecular Dynamics Simulation Methods in Chemistry |

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|---|---|
| • Dates (from – to) | July, 2006 |
| • Name and type of organisation providing education and training | University of Naples Federico II, Naple, Italy |
| • Principal subjects/occupational skills covered | Research stage at the Laboratory of Structure and Dynamics of Molecules, in the group of Prof. Vincenzo Barone |

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| • Dates (from – to) | September 24 - October 2, 2005 |
| • Name and type of organisation providing education and training | Center of Scientific Culture "Ettore Majorana", Erice, Trapani, Italy |
| • Principal subjects/occupational skills covered | International School of Liquid Crystal: Nanoscale Self-Organizing Multifunctional Organic Materials |

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| • Dates (from – to) | September, 7-9, 2005 |

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| • Name and type of organisation providing education and training | University of Padua, Brixen, Italy |
| • Principal subjects/occupational skills covered | National School of Biophysics: Surface and Biosystems |
| • Dates (from – to) | 1999-2004 |
| • Name and type of organisation providing education and training | University of Padua, Padua, Italy |
| • Principal subjects/occupational skills covered | Thesis title: "Modelli diffusivi per fluoroionofori in solventi polari "<br>Advisor: Prof. Antonino Polimeno |
| • Title of qualification awarded | Laurea (M.Sc. equivalent) in Chemistry (specialization in physical chemistry), grade 110/110 |

## TEACHING EXPERIENCES

### *INTERNATIONAL*

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|---|---|
| A.A. 2018 - 2019 | Teacher "Computational Chemistry" (8 hours) Univesitat de Valencia*, V*alencia, Spain (November 2018) |
| A.A. 2017 - 2018 | Teacher "Inorganic Chemistry" (8 hours) Technische Universiteit Eindhoven, Eindhoven, The Netherlands (June 2018) |

### *NATIONAL*

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| A.A. 2019 - 2020 | Teacher in the class of "Fondamenti di Chimica e Educazione Ambientale" (30 hours), academic courses "Laurea in Scienze della Formazione Primaria", University of Padua, Padua, Italy |
| A.A. 2018 - 2019 | Teaching assistance in the class of "Chimica generale e inorganica" (24 hours), academic courses "Laurea in Chimica" "Laurea in Chimica Industriale" and "Laurea in Scienze dei Materiali", University of Padua, Padua, Italy |
| A.A. 2018 - 2019 | Teaching assistance in the class of "Chimica Inorganica 3" (24 hours), academic courses "Laurea Magistrale in Chimica", University of Padua, Padua, Italy |
| A.A. 2018 - 2019 | Teacher in the class of "Fondamenti di Chimica e Educazione Ambientale" (30 hours), academic courses "Laurea in Scienze della Formazione Primaria", University of Padua, Padua, Italy |
| A.A. 2017 - 2018 | Teaching assistance in the class of "Chimica generale e inorganica" (48 hours), academic courses "Laurea in Chimica" "Laurea in Chimica Industriale" and "Laurea in Scienze dei Materiali", University of Padua, Padua, Italy |
| A.A. 2017 - 2018 | Teaching assistance in the class of "Chimica Inorganica 3" (24 hours), academic courses "Laurea Magistrale in Chimica", University of Padua, Padua, Italy |
| A.A. 2016 - 2017 | Teaching assistance in the class of "Chimica generale e inorganica" (72 hours), academic courses "Laurea in Chimica" "Laurea in Chimica Industriale" and "Laurea in Scienze dei Materiali", University of Padua, Padua, Italy |
| Gen 2016 | Teaching in the Computational laboratory at the SMART Winter School (Space-time Multiscale Approaches for Research and Technology), Scuola Normale Superiore, Pisa, Italy. |
| A.A. 2013 - 2014 | Teaching assistance in the class of "Chimica generale e inorganica e chimica fisica" (50 hours), academic course "Laurea in Scienze e tecnologie per l'ambiente", University of Padua, Padua, Italy |
| A.A. 2012 - 2013 | Teaching assistance in the class of "Chimica fisica III" (25 hours), academic course "Laurea triennale in Chimica", University of Padua, Padua, Italy |
| A.A. 2011 - 2012 | Teaching assistance in the classes of "Chimica fisica III" (50 hours), academic course "Laurea in Chimica" University of Padua, Padua, Italy |
| A.A. 2011 - 2012 | Teaching assistance in the classes of "Chimica fisica" (30 hours), accademic course "Laurea in Biotecnologie", University of Padua, Padua, Italy |
| A.A. 2010 - 2011 | Teaching assistance in the class of "Chimica fisica III" (50 hours), academic course "Laurea triennale in Chimica", University of Padua, Padua, Italy |
| A.A. 2009 - 2010 | Teaching assistance in the class of "Chimica fisica III" (50 hours), academic course "Laurea triennale in Chimica", University of Padua, Padua, Italy |
| A.A. 2008 - 2009 | Teaching assistance in the classes of "Chimica fisica III" (50 hours) academic course "Laurea triennale in Chimica", University of Padua, Padua, Italy |
| A.A. 2008 - 2009 | Teaching assistance in the classes of "Chimica Computazionale" (25 hours), academic course "Laurea triennale in Chimica", University of Padua, Padua, Italy |
| A.A. 2007 - 2008 | Teaching assistance in the classes of "Chimica fisica III" (25 hours), academic course "Laurea triennale in Chimica", University of Padua, Padua, Italy |

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| A.A. 2007 - 2008 | Teaching assistance in the classes of "Spectroscopies" (25 hours), accademic course "Laurea triennale in Biotecnologie", University of Padua, Padua, Italy |
| A.A. 2006 - 2007 | Teaching assistance in the class of "Chimica fisica III" (25 hours), academic course "Laurea triennale in Chimica", University of Padua, Padua, Italy |
| A.A. 2005 - 2006 | Teaching assistance in the classes of "Chimica fisica I" (25 hours), academic course "Laurea triennale in Chimica", University of Padua, Padua, Italy |
| A.A. 2005 - 2006 | Teaching assistance in the classes of "Chimica Computazionale" (50 hours), academic course "Laurea triennale in Chimica", University of Padua, Padua, Italy |

## CONFERENCE PARTICIPATION

INVITED SPEAKER

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|---|---|
| 2019 | "3rd International Conference on Catalysis and Chemical Engineering" (Houston, TX, USA, UK, February) |
| 2018 | "5th International Congress on Physical and Theoretical Chemistry" (Edinburgh, UK, October) |
| 2018 | “5th International Congress on Microscopy and Spectroscopy (INTERM)" (Turkey, April) |
| 2017 | “International Conference on Material Science” (Rome, Italy, October) |

ORAL PRESENTATION

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|---|---|
| 2018 | Advanced inorganic materials: green and unconventional synthesis approaches and functional assessment (Padova, Italy, September). |
| 2015 | XLII CONGRESSO NAZIONALE DI CHIMICA INORGANICA (Camerino, Italy, September) |
| 2012 | 4° Forum Nazionale dei Giovani Ricercatori di Scienza e Tecnologia dei Materiali (Padua, Italy, May) |
| 2011 | XXIV Congresso Nazionale della Società Chimica Italiana (Lecce, Italy, September) |
| 2009 | SAMIC 2009 - Syntheses and methodologies in Inorganic Chemistry (Brixen, Italy, December) |
| 2008 | 1° Forum nazionale dei giovani ricercatori di Scienza e Tecnologia dei materiali (Brixen, Italy, November) |
| 2008 | 7th European Conference on Computational Chemistry (San Servolo, Venezia, Italy, September) |
| 2007 | Organic/inorganic hybrid molecular nanostructures for photonic (Padova, Italy, September) |
| 2007 | VI Convegno Nazionale sulla Scienza e Tecnologia dei Materiali (Perugia, Italy, June) |

POSTER PRESENTATION

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| 2013 | 2° Congresso Nazionale della Divisione di Chimica Teorica e Computazionale (Padua, Italy, February) |
| 2012 | 1° Congresso Nazionale della Divisione di Chimica Teorica e Computazionale (Pisa, Italy, February) |
| 2012 | Winter Modeling (Pisa, Italy, February) |
| 2010 | 3° FORUM Nazionale dei Giovani Ricercatori per la Scienza e Tecnologia dei Materiali (Padua, Italy, March) |
| 2010 | Winter Modeling (Pisa, Italy, February) |
| 2009 | Gordon Research Conference on Physics and Chemistry of Microfluidics (Lucca, Italy, July) |
| 2009 | VII Convegno Nazionale INSTM sulla Scienza e Tecnologia dei Materiali (Pisa, Italy, June) |
| 2009 | Lab on a Chip European Congress (Stockholm, Sweden, May) |
| 2009 | TheTIS-Theoretical Tools for in-Silico Spectroscopy (Pisa, Italy, February) |
| 2008 | Winter Modeling (Pisa, Italy, December) |
| 2008 | 4th Japanese-Italian Workshop on Liquid Crystal (JILC2008) (Nara, Japan, July) |
| 2008 | TheTIS-Theoretical Tools for in-Silico Spectroscopy (Paris, France, February) |
| 2007 | SAMIC 2007 - Syntheses and methodologies in Inorganic Chemistry (Brixen, Italy, December) |
| 2007 | 12th International Conference on the Applications of Density Functional Theory (DFT 2007 (Amsterdam, The Netherlands, August) |
| 2007 | EUROMAR 2007 (Tarragona, Spain, July) |
| 2006 | VI Convegno nazionale GICC (Venice, Italy, December) |
| 2006 | 6th European Federation of EPR Groups Meeting (Madrid, Spain, September) |
| 2005 | VII Congress Complex Systems: structure, properties, reactivity and dynamics (Sassari, Italy, June) |

PARTECIPATION

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| 2018 | Spring Meeting Swiss Association of Computational Chemistry (SACC) (Bern, Swiss, February) |
| 2016 | Symposium "La luce di sincrotrone nella chimica e nelle scienze della vita: realtà e prospettive", |

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| | (Padua, Italy, June) |
| 2014 | Winter Modeling (Pisa, Italy, December) |
| 2014 | Italian Grid Training Workshop (Rome, Italy, January) |
| 2011 | Winter Modeling (Pisa, Italy, February) |
| 2010 | Workshop Calcolo scientifico e visualizzazione 3D: nuove prospettive e tecnologie (Bologna, Italy, September) |
| 2008 | 1st European Conference on Microfluidics (μFlu'08) (Bologna, Italy, December) |
| 2007 | One Day Meeting on Inorganic and Hybrid Nanomaterials (Padua, Italy, September) |

## PRINCIPAL INVESTIGATOR

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| September 2017 - September 2019 | Finanziamenti per la Ricerca - Bando 2017- Progetti DiSC (P-DiSC 2017). Project CHIRoN (Computational and syntHetic Investigations on self-assembly cooRdination Nanocapsule) |
| September 2019-July 2020 | ICSRA Project "Theoretical investigation of the dehydroaromatization of methane reaction mechanism catalyzed by Molybdenum (MoCATA)" at the CINECA |

## GRANTS FOR SCIENTIFIC COLLABORATIONS (VISITING RESEARCHER)

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| June 2018 – August 2018 | Bilateral agreements University of Padova / University of Tokyo. Mobilita' di docenti Accordi Bilaterali – Anno 2018, grant from University of Padova, Japanese partner: prof. Yoshitaka Umeno (University of Tokyo) |
| January 2018 – May 2018 | Project "Mechanistic understanding of unusual Ir-carbene reactivity. A DFT Approach", grant from FNDNF (Fonds National Suisse de la Recherche Scientique), Swiss partner: prof. Amalia Isabel Poblador-Bahamonde (Université de Genève). |

## GRANTS FOR RESEARCH ACTIVITIES

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| December 2017 | Grant for "Finanziamento per le attività di ricerca di base". |

## PROJECT PARTICIPATION

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| 2015 - 2016 | Progetto PRAT CPDA134272/13, project $S_3$MArTA "Surface Self-assembled SupraMolecular Architectures, a Theoretically Approach" (prof. M. Casarin) come prestatore di lavoro autonomo occasionale della durata di 4 mesi (periodo 14/12/2015-13/04/2015) (protocollo n. 3503) |
| 2014 - 2015 | Progetto PRAT CPDA134272/13, project S3MArTA "Surface Self-assembled SupraMolecular Architectures, a Theoretically Approach" (prof. M. Casarin) come assegnista di ricerca della durata di 12 mesi (periodo 01/11/2014-31/10/2015) (repertorio n. 139-2014) (protocollo n. 2431) |
| 2012 - 2014 | Progetto Europeo NEXTGENCAT (Development of NEXT GENeration cost efficient automotive CATalysts), Project N° 280890, come assegnista di ricerca della durata di 24 mesi (periodo 01/11/2012-31/10/2014) (repertorio n. 61-2012, protocollo n. 1887) |
| 2012-2016 | Fondi ex 60% (responsabile prof. M. Sambi) |
| 2011 - 2012 | Progetto Strategico di Ateneo HELIOS (Highly Efficient Light Interactions with Organized molecular Systems), coordinatore prof. M. Maggini, come assegnista di ricerca della durata di 12 mesi (periodo 01/11/2011-31/10/2012) (repertorio n.56-2011, protocollo n. 1635) |
| 2011 | PRIN - Bando 2008 dal titolo "Approcci multiscala alle dinamiche molecolari in soluzione" (prof. A. Polimeno) con una borsa di studio per attività di ricerca della durata di 8 mesi (periodo 01/03/2011-31/10/2011) (protocollo n. 432/2011) |
| 2009 - 2011 | Progetto MISCHA (MIcrofluidics laboratory for Scientific and teCHnological Applications), Bando Progetti di Eccellenza 2007-2008 CARIPARO, coordinatore prof. M. Maggini, come assegnista di ricerca della durata di 24 mesi (periodo 01/03/2009-28/02/2011) (repertorio n. 603-2009, protocollo n. 18522) |
| 2008 - 2009 | Progetto FIRB "Composti molecolari e materiali ibridi nanostrutturati con proprietà ottiche |

risonanti e non risonanti per dispositivi fotonici" (prof. R. Bozio) come assegnista di ricerca della durata di 12 mesi (periodo 01/03/2008-28/02/2009) (repertorio n. 608-2008, protocollo n. 15172)

2008 PRIN - Bando 2006 dal titolo "Metodi computazionali per lo studio di proprietà strutturali e dinamiche di nanoparticelle in sospensioni colloidali" (prof. A. Polimeno), contratto di collaborazione coordinata e continuativa per attività di ricerca della durata di 2 mesi (periodo 02/01/2008-29/02/2008) (repertorio n. 38/2007, protocollo n. 1735/07)

2008-2012 Fondi ex 60% (responsabile prof. G. Moro).

## PUBLICATIONS

Il numero di pubblicazioni attualmente riportati su Scopus è 50, il numero di citazioni è 376, mentre l'h-index è pari a 11.

Papers

52 I. Cojocariu, S. Carlotto, H. M. Sturmeit, G. Zamborlini, M. Cinchetti, A. Cossaro, A. Verdini, L. Floreano, M. Jugovac, P. Puschnig, C. Piamonteze, M. Casarin, V. Feyer, C. M. Schneider "Ferrous to ferric transition in Fe-phthalocyanine driven by $NO_2$ exposure". Chemistry – A European Journal, *submitted*.

51 L. Babetto*, S. Carlotto*, A. Carlotto, M. Rancan, G. Bottaro, L. Armelao, M. Casarin, "Antenna triplet DFT calculations to drive the design of luminescent $Ln^{3+}$ complexes", Dalton Transactions, 2020, DOI: 10.1039/D0DT02624G. Corresponding author. (* Equal contribution).

50 P. Machaín, J.D. Fuhr, S. Schneider, S. Carlotto, M. Casarin, A. Cossaro, A. Verdini, L. Floreano, M. Lingenfelder, J.E. Gayone, H. Ascolani, "Mn-Cu Transmetalation as a Strategy for the Assembly of Decoupled Metal-organic Networks on Sn/Cu(001) Surface Alloys", The Journal of Physical Chemistry C, 2020, 124, 35, 18993–19002.

49 A. Carlotto, L. Babetto, G. Bottaro, S. Carlotto, M. Miozzi, M. Rancan, R. Seraglia, M. Casarin, L. Armelao, "Luminescent thermometers: from a library of Eu(III)-β-diketonates to a general model for predicting the thermometric behaviour of europium-based coordination systems", ChemPhotoChem, 2020, 4, 674 - 68.

48 G. Casella, S. Carlotto, M. Mozzon, P. Sgarbossa, R. Bertani, M. Casarin, "A DFT mechanistic study of the synthesis of trans-$[Pt^{II}Cl(NH_3)\{HN=C(NH_2)Me\}_2]Cl$ from addition of $NH_3$ to trans-Z,Z-$[Pt^{II}Cl_2(N{\equiv}CMe)_2]$, Inorganica Chimica Acta, 2020, 511, 119847 (1-8).

47 S. Carlotto, "The role of the dopant and structural defects on the water absorption and on the $H_2$ formation in the Al, Co and Cu doped $SrTiO_3$ perovskite steps", Applied Surface Science, 2020, 527, 146850 (1-7). Corresponding author.

46 S. Carlotto, A. Vittadini, M. Casarin, "DFT modelling of the NO reduction process at the Cu-doped $SrTiO_3$(100) stepped surface", Inorganica Chimica Acta, 2020, 511, 119813 (1-7). Corresponding author.

45 S. Carlotto, A. Vittadini, M. Casarin, "DFT modelling of the CO-NO redox reaction at Cu-doped $SrTiO_3$(100) stepped surface: CO oxidation at lattice O ions", Inorganica Chimica Acta, 2020, 511, 119810 (1-6). Corresponding author.

44 S. Carlotto, A. Glisenti, A. Vittadini, M. Casarin, "Adsorption and reactivity of CO at a stepped $SrTiO_3$(1 0 0) surface in the presence of Cu impurities", Applied Surface Science, 2020, 521, 146450 (1-5). Corresponding author.

43 F. Sedona, M.M. Seyyed Fakhrabadi, S. Carlotto, E. Mohebbi, F. De Boni, M. Casarin, M. Sambi, "On-surface synthesis of extended linear graphyne molecular wires by protecting the alkynyl group", Physical Chemistry Chemical Physics, 2020, 22, 12180-12186.

42 S. Carlotto, E. Mohebbi, F. Sedona, M. Lo Cicero, L. Colazzo, C. Mariani, M.G. Betti, M. Sambi, M. Casarin, "An experimental and theoretical study of metallorganic coordination networks of tetrahydroxyquinone on Cu(111)", New Journal of Chemistry, 2019, 43, 19186-19192. Corresponding author.

41 S. Carlotto, P. Finetti, M. de Simone, M. Coreno, G. Casella, M. Sambi, M. Casarin,

"Comparative Experimental and Theoretical Study of the C and O K-edge X-ray Absorption Spectroscopy in Three Highly Popular, Low Spin Organoiron Complexes ([$Fe(CO)_5$], [($\eta_5$-$C_5H_5$)Fe(CO)(μ-CO)]$_2$ and [($\eta_5$-$C_5H_5$)$_2$Fe])", Inorganic Chemistry, 2019, 58, 16411-16423. Corresponding author.

40 S. Carlotto, A. Bonna, K. Bossak-Ahmad, W. Bal, M. Porchia, M. Casarin, F. Tisato, "Coordinative unsaturated $Cu^I$ entities are crucial intermediates governing cell internalization of copper. A combined experimental ESI-MS and DFT study", Metallomics, 2019, 11, 1800-1804. Corresponding author.

39 G. Casella, C. Fonseca Guerra, S. Carlotto, P. Sgarbossa, R. Bertani, M. Casarin, "New light on an old debate: does the RCN–$PtCl_2$ bond include any back-donation? RCN←$PtCl_2$ backbonding *vs.* the IR $\nu_{C\equiv N}$ blue-shift dichotomy in organonitriles–platinum(II) complexes. A thorough density functional theory–energy decomposition analysis study", Dalton Transactions, 2019, 48, 12974-12985.

38 S. Carlotto, G. Casella, L. Floreano, A. Verdini, A.P.C. Ribeiro, L.M.D.R.S. Martins, M. Casarin, "Spin State, Electronic Structure and Bonding on C-Scorpionate [Fe(II)$Cl_2$(tpm)] Catalyst: an Experimental and Computational study", Catalysis Today, 2019, DOI : 10.1016/j.cattod.2019.08.010. Corresponding author.

37 S. Carlotto, P. Finetti, M. de Simone, M. Coreno, G. Casella, M. Sambi, M. Casarin, "Comparative Experimental and Theoretical Study of the Fe $L_{2,3}$-Edges X-ray Absorption Spectroscopy in Three Highly Popular, Low-Spin Organoiron Complexes: [$Fe(CO)_5$], [($\eta^5$-$C_5H_5$)Fe(CO)(μ-CO)]$_2$, and [($\eta^5$-$C_5H_5$)$_2$Fe]", Inorganic Chemistry, 2019, 58, 5844-5857. Corresponding author.

36 S. Carlotto, "Transition metail systems: a theoretical modeling of their $L_{2,3}$-edge X-ray absorption spectra", Journal of Physical Chemistry & Biophysics, 2018, 8, 86. Corresponding author.

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5 S. Carlotto, M. Casarin, A. Lanza, F. Nestola, L. Pandolfo, C. Pettinari, R: Scatena "Reaction of Copper(II) Chloroacetate with Pyrazole. Synthesis of a 1D Coordination polymer and unexpected dehydrochlorination reaction”, Atti del XLII CONGRESSO NAZIONALE DI CHIMICA INORGANICA, ISBN: 9788867680238, Camerino, 9-12 Sept. 2015.

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Other publications

4 S. Carlotto,
"L’ascesa al Principio e la discesa: Platone e Plotino a confronto "
Tesi di Laurea di Laure Magistrale in Scienze Filosofiche, 2011
Codice identificativo: IT\ICCU\VIA\0240866, Codice SBN: VIA0240866

3 S. Carlotto,
"Il mito di Er nel libro X della *Repubblica* di Platone"
Tesi di Laurea Triennale in Filosofia, 2008

2 S. Carlotto,
"Modeling of dynamic solvation effects"
Tesi di Dottorato in Scienze Molecolari, 2008

1 S. Carlotto,
"Modelli diffusivi per fluoroionofori in solventi"
Tesi di Laurea in Chimica, 2004

## EDITORIAL STAFF

Topic Editor for *Molecules*
Topic Editor for *Chemosensors*

## CULTORE DELLA MATERIA

Cultore della materia per il SSD CHIM/03

## SCIENTIFIC COMMITTEE MEMBER

2019 "World Congress on Chemistry (WCC-2019)" (Valencia, Spain, October)
2018 “5th International Congress on Microscopy and Spectroscopy (INTERM)" (Turkey, April)

## ORGANIZING COMMITTEE MEMBER

2021 “International Conference on Chemistry” (Amsterdam, Netherlands, April).
2021 “International Conference on Physics and Space Sciences” (Osaka, Japan, March)
2020 "International Conference on Physics and Networks” (Seoul, South Korea, June)
2019 "World Congress on Chemistry (WCC-2019)" (Valencia, Spain, October)
2019 "2rd World Congress on Chemistry" (Rome, Italy, October).
2018 “World Congress of chemistry" (Rome, Italy, November)

## ADDITIONAL INFORMATION

Current

Reviewer of international scientific journal such as "Physical Chemistry Chemical Physics", "International Journal of Molecules Sciences", “Molecules”, “International Journal of Molecular Sciences”, "Dalton Transactions", "Journal of Molecular Modeling", "International Journal of Heat and Mass Transfer", "Journal of Physical Chemistry", "Journal of Material Chemistry C", "Journal of Chemical Educational", "Journal of Physics and Chemistry of Solids", “International Journal of Environmental Research and Public Health”, “Brazilian Journal of Chemical Engineering”, "Antioxidants".
Reviewer of ISCRA (Italian SuperComputing Resource Allocation) international project at the CINECA.

## COLLABORATIONS

| | |
|---|---|
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## PERSONAL SKILLS AND COMPETENCES

| | |
|---|---|
| MOTHER TONGUE | **ITALIAN** |
| OTHER LANGUAGE | |
| **ENGLISH** | good |
| SOCIAL SKILLS AND COMPETENCES | 2017, 2016, 2015, 2011, 2010, 2009, 2008: Scientific divulgation activities at the Department of Chemical Sciences, University of Padua, Padua, Italy<br>2016: Scientific divulgation activities at Padua (Istituto Nazionale di Fisica Nucleare and CNR) |
| ORGANISATIONAL SKILLS AND COMPETENCES | Sense of responsibility and initiative<br>Highly organized<br>Excellent planning skills with great attention to detail and ability to prioritize work<br>Team worker with good initiative and problem-solving attitude<br>Negotiation and time management skills |
| COMPUTER SKILLS AND COMPETENCES | Experienced in the usage of operating systems (Windows, Linux and OsX)<br>Basic knowledge in programming languages (Fortran and C++)<br>GAUSSIAN, DALTON, ADF and ORCA for quantum mechanical approaches<br>QuantumESPRESSO for quantum mechanical calculations (periodic systems)<br>AMBER e LAMMPS for molecular dynamics calculations<br>COMSOL for macroscopic approaches |

Padova, 29th September 2020