Curriculum Vitae

Alessandra Magistrato

Career

June 2006 –present	Permanent position as researcher at CNR-IOM hosted by the International School for Advanced Studies (SISSA), Trieste, Italy.
Jan 2003 – June 2006	Tenure Track position at CNR-INFM-Democritos National Simulation Center hosted by International School for Advanced Studies (SISSA), Trieste, Italy.
Jul 2001 - Dec 2002	Postdoctoral Fellow at the Chemistry Department, University of Pennsylvania, Philadelphia, PA, USA (Prof. M. L. Klein's group).

Teaching assignments

2016-2018 Professor at SISSA for PhD in 'Physics and Chemistry of Biological System'

Qualifications

2012 Associate Professor in General and Inorganic Chemistry (2013-2022)
2014 Associate Professor of General and Clinical Biochemistry (2014-2022)
2014 Associate Professor in Theoretical Physics of Matter (2013-2022) (03/B2)
2018 Associate Professor of Physical Chemistry (2018-2022)
2018 Full Professor in General and Inorganic Chemistry (2018-2022)
2018 Full Professor of General and Clinical Biochemistry (2018-2022)
2018 Full Professor in Theoretical Physics of Matter (2018-2022)
2018 Full Professor of Physical Chemistry (2018-2022)

Education

April 2001	PhD degree ETH Zentrum, Zürich, Switzerland.
1998–2001	PhD in Computational Inorganic Chemistry, in the group of Prof. U. Röthlisberger, ETH Zentrum, Zürich, Switzerland.
November 1997	Graduated *"cum laude"* at the University of Perugia, Italy.
1992–1997	Undergraduate Student of Chemistry (*Physical Chemistry*) at the University of Perugia, Italy.

Leaves Periods

April 2009-May 2010	Maternity leave
November 2011-November 2012	Maternity leave

Publications

Author of 66 articles, 4 book chapters, 8 Conference Proceedings
H-index: 26 (font Google Scholar, January 2018) Citations: 1808

Supervision Experience
2004-2017 supervisor of
10 *PhD students*: Attilio Vargiu (2004-2008, SISSA), Fabio Simona (2005-2008, SISSA), Giulia Rossetti (2006-2010, SISSA), Rolando Hong (2005-2009, SISSA), Duvan Franco (2009-2014, SISSA), Ina Bisha (2011-2014)), Federica De Leo (2010-2014, University of Namur), Lorenzo Casalino (2013-2017, SISSA), Maria Letizia Merlini (2016-EPFL, Lausanne), Mariami Rushvili (2016-2018, SISSA), Andrea Saltalamacchia (2017-)

9 *postdocs*: Aneta Jezierska (2008), Arturo Robertazzi (2006-2008), Branimir Bertosa (2008-2009), Jacopo Sgrignani (2010-2012), Angelo Spinello (2016-), Matic Pavlin (2016-), Ida Ritacco (2017-), Jure Borisek (2017-2018), Fabio Doro (2018-)

3 *bachelor students*: Marta Bon (February-November 2013), Nadira Abdurakhmanova (2013-2015), Andrea Saltalamacchia (2017).

Grants
Projects as PI

POR-FESR 2014-2020 'ARES' Against Brain Cancer: Finding personalized therapies with in silico and in vitro studies' (210000 €) *2018-2021*

Talents 3-FVG Fellowship 'Disclosing the molecular mechanism of the eukaryotic spliceosome with molecular simulations' 2017-2018 (40.230 €)

'My first AIRC grant: *Starting grant for your researchers (under 40 years old) from the Italian Cancer Research Association* (AIRC) 'Learning the lesson of tamoxifen metabolites design of multi targeted human aromatase and estrogen receptor modulators' (220000 €) financed by AIRC 2016-2018

AIRC fellowships 'Gianni Bonadonna' 'Molecular Switchers of Aromatase: the Next-Generation Inhibitors Targeting a Phosphorylation Site at the Cytochrome Reductase Interface' 2016-2017 (90000 €)

Project of cooperation Italy-Israel 'Disclosing Interactions Between Copper Cellular Transporters: Toward New Treatments for Copper Metabolism Dysfunctions' 2017-2019, (€145.681,9)

Project founded by 'Fondo sociale europeo della regione Friuli venezia giulia 2007/2013' PhD fellowship cofinancing for the period 1/1/2014-30/6/2015

PhD fellowship funded by MIUR 'Fondo per il Sostegno dei Giovani e per favorire la mobilità degli studenti" istituito con Decreto Ministeriale MIUR 198/2003' hosted by SISSA (2011)

BANDO PER LA RACCOLTA DI PROGETTI CONGIUNTI DI RICERCA SCIENTIFICA E TECNOLOGICA PER IL PERIODO 2008-2009 NELL'AMBITO DEL PROGRAMMA DI COLLABORAZIONE SCIENTIFICA E TECNOLOGICA TRA ITALIA E ARGENTINA PER IL PERIODO 2008-2009, 'The Role of Copper in α-synuclein and Parkinson's Disease' in collaboration with Prof. C.O. Fernandez, University of Rosario, Argentina. (Cover for travel expenses for the exchange visits of the researchers).

Recipient of Swiss National Science Foundation grant for postdoc at University of Pennsylvania, Philadelphia, PA, USA (2001-2002).

Project as Partecipant
'Nanoscience Foundries and Fine Analysis' Founded by Horizon 2020 (2015-2019) (2758161 €).

NANOCANCER Project funded by Regione Friuli Venezia Giulia headed by the University of Trieste (30,000 €).

COFIN 2008 'Computational Studies of the Cu(II) and Zn(II) Role in the Neurotrophin/Receptor Complex Formation and Design of Neurotrophin Mimetic Peptides' Headed by Prof. Rizzarelli, University of Catania (€ 1120000)

PROGRAMMI PER L'INCENTIVAZIONE DEL PROCESSO DI INTERNAZIONALIZZAZIONE DEL SISTEMA UNIVERSITARIO, COLLABORAZIONI INTERUNIVERSITARIE INTERNAZIONALI (2004-2006), 'Study of Enzymatic Activity and Inhibition of Metallo-b-Lactamases via Computer Simulation Techniques' (€10,000)

PROGETTO MAE between SISSA/DEMOCRITOS and Instituto de Investigacion en Fisico Quimica de Cordoba-Argentina, 'Study of Enzymatic Activity and Inhibition of Metallo-b-Lactamases via Computer Simulation Techniques' for the period 2006-07 (€10,000).

Project art. 11 of L.R. 11/2003 'New Therapies and Drugs in Antitumoral Drugs: Inorganic Antimetastatic Drugs, Genetic Therapy and Nanobiotechnologies'. Headed by the University of Trieste (Prof. M. Prato). For the period: 01/10/2006-30/09/2007 (€ 30,000).

Project art. 11 of L.R. 11/2003 Title 'New Antitumoral Technologies'. Headed by the University of Trieste (Prof. M. Prato). For the period 01/10/2008-30/09/2009 (€ 30,000)

Grants for Computing

2017 PI of 3 ISCRA grants for computer time at CINECA on IBM-blugene, and Marconi Bologna, Italy (hrs) 550000 core hrs on Marconi

2012-2016 PI of 6 ISCRA grants for computer time at CINECA on IBM-blugene, and Marconi Bologna, Italy (48 millions hrs)

2010-2012 PI of 4 ISCRA grants for computer time at CINECA on sp6 machine, Bologna, Italy (600,000 hrs)

2010-2012 PI of 3 grants at CASPUR (300,000 hrs)

PI of 20 grants for computer time given by INFM (Italian Institute for condensed matter theory) in the CINECA supercomputing center in Bologna: distributed on a cluster Linux (Beowulf) and on IBM- sp3,sp4,sp5 and on cluster of opteron dual core processors in the period 2003-2009.

Co-PI of 2 Grants by the Distributed European Infrastructure for Supercomputing Applications (DEISA) Extreme Computing Initiative (400,000 hours on IBM sp5).

Peer Reviewer Activity

Funding Agencies

Panel Member PRACE infrastructure (Life Science)

Referee

Journals

Structure, Journal of Physical Chemistry B, Chemistry A European Journal, New Journal of Chemistry, Organic Biomolecular Chemistry, Inorganic Chemistry, Organometallics, Proteins, ChemPhysChem, J. Am. Chem. Soc., Theoretical Chemistry Accounts, Journal of Chemical Theory and Computation, Proteins: Structure, Function and Bioinformatics, ACS Catalysis, Journal of Inorganic Biochemistry, Chemical Physics Letters. Angewante Chemie, Journal of Chemical Information and Modeling, Chemical Review, Plos Computational Biology

Funding Agencies

Swiss National Science Foundation, National Science Foundation, USA, Croatian Science Foundation, PRACE Infrastructure, Italian-French University, Austrian Science Foundation, French National Science Foundation, Dutch National Science Foundation, ANVUR-MIUR, PRACE Infrastructure

External examiner PhD commissions

EPFL Lausanne (February 2014, February 2016), University of Namur, Belgium (January 2015), University of Cagliari (May 2015), University of Calabria (December 2015), EPFL July 2017, EPFL September 2017.

Teaching Experience

2018-2019 ‘Introduction to Biochemistry’ (40 hrs, SISSA, Teaching assignment)

2017-2018 ‘Introduction to Biochemistry’ (40 hrs, SISSA, Teaching assignment)

2016-2017 ‘Introduction to Biochemistry’ (40 hrs, SISSA, Teaching assignment)

2014-2016 Lectures on ‘Simulation in molecular medicines’ (SISSA, Italy)

2011 Lectures on ‘Simulation in molecular medicines’ and ‘Principles of Quantum Chemistry'. (SISSA, Italy)

2003-2008 Annual series of lectures and exercises in ‘Principles of Quantum Chemistry' (SISSA, Italy).

2000-2001 and 1999-2000 October-March teaching assistantship position for Inorganic Chemistry Laboratory at the (ETH Zentrum, Zürich, Switzerland).

January 2000 Lectures in theoretical inorganic chemistry (ETH Zentrum, Zürich, Switzerland.

2007 Lectures and Exercises of molecular dynamics simulations at the ICTP conference ‘Drug Development for the Third World’.

2005-2006 Summer School Molecular Design and Computer Aided Chemistry ICS-UNIDO ‘Principles of Quantum Chemistry’, Trieste, Italy.

2005 Summer School ‘Biomath: Modelling of Biological Systems', in Trieste.

Invited Talks

‘Computational Adavnces in Drug Discovery’ Sestri Levante (GE) September 2019

CECAM ‘Ions, membranes and channels: multiscale simulations from quantum to coarse-grain. A symposium in honor of Mike Klein’s 80th birthday.’ Paris, France March 2020

CPMD Meting 2018 Lausanne, Switzerland, 22-24th, in July 2019

CECAM Conference ‘Multiscale Modeling from Macromolecules to Cell: Opportunities and Challenges of Biomolecular Simulations’ *Lausanne, Switzerland February 4- 6, 2019*

Bar-Ilan University, Tel Aviv, Israel November 5th 2018

CECAM conference ‘Multiscale modelling in electrophysiology: from atoms to organs" Lugano (Switzerland) 26-28th March 2018

CECAM conference 'Physiological role of ions in the brain: towards a comprehensive view by molecular simulation' Pisa May 21st-23rd 2018

University of Heidelberger, December 14th 2017

National Institute of Chemistry, Ljubljana, Slovenia November 21th 2017

Computational Advances in Drug Discovery, Lausanne, CH September 5th-8th, 2017

ACS Meeting Symposium 'New Paradigm for Catalyst Design: From Enzymatic Function to Functional Mimics' Washington DC, USA August 20th-24th, 2017.

University of Bologna, Bologna April 28th 2017

25th Croatian Meeting of Chemists and Chemical Engineers, Porec, Croatia 19th – 22nd of April 2017

CNR-ICRM Milano November 15th 2016

Deutche Zentrum Fuer Neurodegenerative Enkrankungen, Bonn, Germany, 23th September 2016

University of Ljubljana, Slovenia, May 9th 2016

University of Calabria, Cosenza IT December 10th 2015

Juelich Forchungzentrum, Juelich Germany July 2nd 2015

Symposium in honor of Ruth Nussinov, Aachen University 22 October 2015

Juelich Forchungzentrum, Juelich Germany July 2nd 2015

CECAM Worshop 'Modeling activity vs. selectivity in metalloproteins' June 29, 2015 to July 1, 2015

Institute for research in Biomedicine, Bellinzona, CH April 2015

University of Namur, Belgium, January 20th 2015,

CECAM Workshop Advanced modeling to investigate biomolecules, November 20-21st 2014 IIT Genova, Italy

University of Wien BOKU, October 9th 2014

EPFL, Lausanne, Switzerland, February 14th 2014

Technical University of Graz, Graz, Austria December 11th 2013

CPMD Meeting 2011, Barcelona, Spain, September 5th-9th, 2011

IOM Workshop Trieste, Trieste, Italy September 30th-October 1st, 2010

Ab initio Modeling In Applied Biosciences, Structure, Dynamics and Function, December 12th 2008 Uppsala, Sweden

King's College, London, UK April 23rd 2008

University of Rosario, Rosario, Argentina, December 21st 2007,

AIMECS 2007, Istanbul, Turkey, July 11st 2007

SIGEA Meeting, Milan, November, 14th, 2006

ACS 2006, San Francisco, CA, USA, September, 12nd, 2006

Conference on Progresses in ab initio modeling of biomolecules, July, 3rd, 2006, Leiden, The Netherlands

University of Wien, Wien, Austria, May 3rd 2006

University of Leiden, Leiden the Netherlands, November 14th 2005

Psi-k 2005, Schwabish Gmund, Germany, September, 18-21th, 2005,

CESAR-COST Meeting, Wien, Austria, July, 7-9th, 2005,

ACS 2005 National Meeting San Diego, CA, USA, March, 13-17th, 2005

University of Trieste, Trieste Italy, September, 28th 2005

University of Cagliari, Cagliari, Italy September 27th, 2004

University of Pennsylvania, Philadelphia, PA, USA. April 6th 2004,

CMS Workshop 2004 Geremeas, CA, Italy, September 18-23rd

ICTP-INFM Conference on New frontiers in nano-biotechnology: monitoring protein function with single protein resolution Trieste, Italy July 14-19th 2003

ETH Zentrum October 25th 2001, Zürich Switzerland,

Emory University, March 22nd 2000, Atlanta, GA, USA

Princeton University, March 15th 2000, Princeton, NJ, USA

List of Peer Reviewed Publications (*corresponding author)

L Casalino, G Palermo, A Spinello, U Rothlisberger, A MagistratoAll-atom simulations disentangle the functional dynamics underlying gene maturation in the intron lariat spliceosome PNAS USA 2018

A Spinello, M Pavlin, L Casalino, A MagistratoA Dehydrogenase Dual Hydrogen Abstraction Mechanism promotes Estrogen Biosynthesis. Can we Expand the Functional Annotation of the Aromatase Enzyme? Chem Eur J 2018

Rusishvili M, Grisanti L, Laporte S, Micciarelli M, Rosa M, Robins R, Collins T, Magistrato A, Baroni S 'Unraveling the molecular mechanisms of color expression in anthocyanins' submitted

Borišek, J, Saltalamacchia, A; Palermo, G; Magistrato, A* Disclosing the impact of carcinogenic SF3b mutations on pre-mRNA recognition via atomic-level simulations submitted

Spinello, A; Martini, S; Berti, F; Pennati, M; Pavlin, M; Sgrignani, Jacopo; Grazioso, G; Colombo, G; Zaffaroni, N; Magistrato, A* A New Generation of Estrogen Biosynthesis Modulators Lays the Foundation for Unprecedented Therapeutic Strategies to Fight Breast Cancer" (submitted)

A Spinello, I Ritacco, Magistrato A* 'Steroidogenic cytochromes P450: the catalytic mechanism, its entwined membrane-induced- and post-transcriptional-modulation as elucidated from atomic-level studies (invited review) Catalyst Submitted

Sgrignani J, Casalino L, Doro F, Spinello A, Magistrato A* "Can Multi-Scale Simulations Unravel the Function of Metallo-Enzymes to Improve Knowledge-based Drug Discovery?" Future Med Chem 2018 submitted

A Spinello, E Vecile, A Dobrina, A Magistrato* "How Can Interleukin-1 Receptor Antagonist Modulate Distinct Cell Death Pathways?" J Chem Info Mod 2018

M Pavlin, A Spinello, M Pennati, N Zaffaroni, S Gobbi, A Bisi, G Colombo, Magistrato A* A Computational Assay of Estrogen Receptor α Antagonists Reveals the Key Common Structural Traits of Drugs Effectively Fighting Refractory Breast Cancers Scientific reports 2018 8 (1), 649

A Magistrato* Direct in silico visualization of ligands channelling through proteins: The next-generation frontier of computational biology. Physics of life reviews 2017, 22, 82

A Spinello, A Magistrato* An Omics Perspective to the Molecular Mechanisms of Anticancer Metallo-drugs in the Computational Microscope Era *Expert Opinion on Drug Discovery* 2017 Aug;12(8):813-825. doi: 10.1080/17460441.2017.1340272

Magistrato, A*.; Sgrignani, J.; Krause, R.; Cavalli A.; Single or multiple access channels to the CYP450s active site? An answer from free energy simulations of the human aromatase enzyme. *J Phys Chem Lett 2017*8 (9), 2036-2042

Casalino L., Palermo G., Abdurakhmonova N., Rothlisberger U., Magistrato A.* 'Development of Site-specific Mg^{2+}-RNA force field parameters: a Dream or a Reality? Guidelines from combined Molecular Dynamics and Quantum Mechanics Simulations' *J. Chem. Theor. Comput.* (2017) 13 (1), 340-352

Casalino L., Palermo G., Rothlisberger U., Magistrato A.* 'Who Activates the Nucleophile in Ribozyme Catalysis? An Answer from the Splicing Mechanism of Group II Introns' *J. Am. Chem. Soc.* (2016) 138 (33), 10374–10377 (Cover Picture)

Casalino L., Magistrato A.* 'Structural, dynamical and catalytic interplay between Mg2+ ions and RNA. Vices and virtues of atomistic simulations' *Inorganica Chimica Acta* (2016) 452, 73-81

Sgrignani J., Cavalli A., Colombo G., Magistrato A.* 'Enzymatic and Inhibition Mechanism of Human Aromatase (CYP19A1) Enzyme. A Computational Perspective from QM/MM and Classical Molecular Dynamics Simulations.' *Mini. Rev. Med. Chem.* (2016) 16(14):1112-24.

Bisha I., Magistrato A.* 'The molecular mechanism of secondary sodium symporters elucidated through the lens of the computational microscope' *RSC Advances* (2016) 6 (12), 9522-9540

Palermo G., Magistrato A., Riedel T., Von Erlach T., Davey CA., Dyson PJ., Rothlisberger U. 'Fighting Cancer with Transition Metal Complexes: From Naked DNA to Protein and Chromatin Targeting Strategies' ChemMedChem (2016) 20,11(12):1199-210

Sgrignani J., Iannuzzi M., Magistrato A.* 'Role of Water in the Puzzling Mechanism of the Final Aromatization Step Promoted by the Human Aromatase Enzyme. Insights from QM/MM MD Simulations' *J. Chem. Info. Mod.* (2015) 55 (10), 2218-2226

Napolitano L. M. R., Bisha I., De March M., Marchesi A., Arcangeletti M., Demitri N., Mazzolini M., Rodriguez A., Magistrato A., Onesti A., Laio A., Torre V. 'Pore flexibility underlies the poor selectivity of CNG channels: a structural, functional and computational analysis. ' *Proc. Natl. Acad. Sci. USA (*2015) 112 (27), E3619-E3628

Sgrignani J., Magistrato A* ’QM/MM MD simulations on the enzymatic pathway of the human flap endonuclease (hFEN1) elucidate common cleavage pathways to RNase H enzymes. ’ *ACS Catalysis* (2015), 5 (6), 3864–3875

Deleo F., Magistrato A., Bonifazi D. **’**Interfacing Proteins with Graphitic Nanomaterials: from Spontaneous Attraction to Tailored Assemblies**’** *Chem. Soc. Rev.* (2015) 44 (19), 6916-6953

Bisha I., Rodriguez A., Laio A., Magistrato A.* ‘Metadynamics Simulations Reveal a Na+ Independent Exiting Path of Galactose for the Inward-Facing Conformation of vSGLT’ *PLOS Comput. Biol.* 10 (12), e1004017 (2014)

Sgrignani J., Bon M., Colombo G., Magistrato A.* ‘Computational Approaches Elucidate the Allosteric Mechanism of Human Aromatase Inhibition: A Novel Possible Route to Small-Molecule Regulation of CYP450s Activities?’ *J. Chem. Info Mod.* (2014) 54 (10), 2856-2868

Franco D., Vargiu AV., Magistrato A.* ‘Ru [(bpy) 2 (dppz)] 2+ and Rh[(bpy)2(chrysi)] 3+ targeting double strand DNA: The shape of the intercalating ligand tunes the free energy landscape of deintercalation’ *Inorg. Chem.* (2014) 53 (15), 7999-8008

Vidossich P., Magistrato A.* ’QM/MM Molecular Dynamics Studies of Metal Binding Proteins’ *Biomolecules* (Invited review Special issue on Metal Binding Proteins) (2014), 4 (3), 616-645.

Vargiu AV., Magistrato A* ’Atomistic‐Level Portrayal of Drug–DNA Interplay: A History of Courtships and Meetings Revealed by Molecular Simulations' *ChemMedChem* Invited review for the special issue on DNA/RNA (2014) 9 (9), 1966-1981

De Leo F., Sgrignani J., Bonifazi D., Magistrato A.* ‘Structural and dynamical properties of monoclonal antibodies immobilized on CNTs: a molecular simulation study’ *Chem. Eur. J.* (2013) 19 (37), 12174-12174 (Cover Picture).

Franco, D., Sgrignani, J., Bussi, G., Magistrato A.* ‘The Structural Role of Uracil DNA Glycosylase for the Recognition of Uracil in DNA duplexes. Clues from Atomistic Simulations’ (2013) *J. Chem. Info. Mod.* 53 (6), 1371–1387 (Cover Picture).

Marega, R., De Leo, F., Pineux, F., Sgrignani, J., Magistrato, A., Naik, A.D., Garcia Y., Flamant, L., Michiels, C., Bonifazi D ‘Functionalized Fe‐Filled Multiwalled Carbon Nanotubes as Multifunctional Scaffolds for Magnetization of Cancer Cells’ *Adv. Funct. Mat.* (2013) 23 (25), 3173-3184 (Cover Picture).

Bisha, I., Laio, A., Magistrato, A.*, Giorgetti, A., Sgrignani J. ‘A Candidate Ion-Retaining State in the Inward-Facing Conformation of Sodium/Galactose Symporter: Clues from Atomistic Simulations’ *J. Chem. Theor. Comput.* (2013) 9 (2), 1240-1246.

Sgrignani J., Magistrato A.* 'First Principles Modeling of Biological Systems and Structure- Based Drug-Design' *Curr. Comput. Aided. Drug. Des.* (2013) 52 (6), 1595-1606 (Invited review).

Sgrignani J., Magistrato A. 'Influence of the Membrane Lipophilic Environment on the Structure and on the Substrate Access/Egress Routes of the Human Aromatase Enzyme' A Computational Study *J. Chem. Inf. Mod.* (2012) 52 (6), 1595-1606 (Cover Image).

Sgrignani J, Magistrato A*, Dal Peraro M, Vila AJ, Carloni P, Pierattelli R. On the active site of mononuclear B1 metallo β-lactamases: a computational study. *J. Comput. Aided Mol. Des.* (2012) 26 (4), 425-435.

Sgrignani J., Magistrato A.* 'The Structural Role of Mg2+ Ions in a Class I RNA Polymerase Ribozyme: A Molecular Simulation Study'*J. Phys. Chem B*, (2012) 116, 7, 2259-2268.

Vargiu A. V., Magistrato A. 'Detecting DNA Mismatches with Metallo-Insertors: A Molecular Simulation Study *Inorg. Chem.* (2012) 51, 4, 2046-2057.

Sgrignani J., Franco D., Magistrato A*. 'Theoretical Studies of Homogeneous Catalysts Mimicking Nitrogenase' *Molecules* (2011) 16, 1, 442-465 (Invited review).

Binolfi A., Rodriguez E. E., Valensin D., D'Amelio N., Ippoliti E., Obal G., Duran R., Magistrato A., Pritsch O., Zweckstetter M., Valensin G., Carloni P., Quintanar L., Griesinger C., Fernández C.O. 'Bioinorganic Chemistry of Parkinson's Disease: Structural Determinants for the Copper-Mediated Amyloid Formation of Alpha-Synuclein' *Inorg. Chem.* (2010) 49, 22, 10668-10679.

Musiani F., Bertosa B., Magistrato A., Zambelli B., Turano P., Losasso, V., Micheletti C., Ciurli S., Carloni P. 'Computational Study of the DNA-Binding Protein Helicobacter pylori NikR: The Role of Ni(2+)' (2010) *J. Chem. Theor. Comput.* 11, 3285, 3503-3515.

Rossetti G., Magistrato A.,* Pastore A., Carloni P. 'Hydrogen Bonding Cooperativity in polyQ beta-Sheets from First Principle Calculations' (2010) *J. Chem. Theor. Comput.* 6, 6, 1777-1782 (Cover Image).

Simona F., Magistrato A., Dal Peraro M., Vila A.J., Carloni P. 'Common mechanistic features in B1 and B2 Metallo-beta-Lactamases: A computational study on Aeromonas hydrophila CphA' (2009) *J. Biol. Chem.* 284, 41, 28164-28171.

Robertazzi A., Vargiu A., Magistrato A.*, Ruggerone P., Carloni P., de Hoog P., Reedijk J. 'Copper-1,10-Phenanthroline Complexes Binding to DNA: Structural Predictions from Molecular Simulations' *J. Phys. Chem B* (2009) 113, 31, 10881-10890.

Brancia F.L., Stener M., Magistrato A. 'A Density Functional Theory (DFT) Study on Gas-Phase Proton Transfer Reactions of Derivatized and Underivatized Peptide Ions

generated by Matrix-assisted Laser Desorption Ionization' *J. Am. Soc. Mass Spectr.* (2009) 20, 7, 1327-1333.

Sooambar C., Troiani V., Bruno C., Marcaccio M., Paolucci F., Listorti A., Belbakra A., Armaroli N., Campagnolo M., Geremia S., Magistrato A., Prato M., Bonifazi D. 'Synthesis, Photophysical, and Electrochemiluminescent Properties of 5,15-Bis(9-antracenyl)porphyrins Derivatives' *Org. Biomol. Chem.,* (2009) 7, 11, 2402-2413

Hong R., Magistrato A.*, Carloni P. 'Anthrax Lethal Factor Investigated by Molecular Simulations' (2008) *J. Chem. Theor. Comput.*, *4*, 1745–1756

Vargiu A.V., Ruggerone P., Magistrato A., Carloni P. 'Dissociation of Minor Groove Binders from DNA: Insights from Metadynamics Simulations.' *Nucleic Acids Res.* (2008) 36, 5910-5921

Rossetti G., Magistrato A.*, Pastore A., Persichetti F., Carloni P. 'Structural Properties of Polyglutamine Aggregates Investigated via Molecular Dynamics Simulations.' *J Phys Chem B*. (2008) 112, 16843-16850

Vargiu A.V., Robertazzi A., Magistrato A.*, Ruggerone P., Carloni P. 'The Hydrolysis Mechanism of the Anticancer Ruthenium Drugs NAMI-A and ICR Investigated by DFT-PCM Calculations.' *J Phys Chem B*., (2008) 112, 4401-4409

Otyepka M., Banás P., Magistrato A., Carloni P., Damborský J. 'Second Step of Hydrolytic Dehalogenation in Haloalkane Dehalogenase Investigated by QM/MM Methods' *Proteins* (2008) 70, 707-717

Vargiu A.V., Ruggerone P., Magistrato A., Carloni P. 'Sliding of Alkylating Anticancer Drugs along the Minor Groove of DNA: New Insights on Sequence Selectivity' *Biophys. J.* (2008) 94, 1-12

Spiegel K., Magistrato A*, Maurer P., Ruggerone P., Rothlisberger U., Carloni P., Reedijk J., Klein M. L. 'Parameterization of Azole-Bridged Dinuclear Platinum Anticancer Drugs via a QM/MM Force Matching Procedure' *J Comput. Chem.* (2008) 29, 38-49

Spiegel K., Magistrato A*, Carloni P., Reedijk J., Klein M. L. 'Azole-Bridged Diplatinum Anticancer Compounds. Modulating DNA Flexibility to Escape Repair Mechanism and Avoid Cross Resistance' *J. Phys. Chem. B* (2007) 111, 11873-11876

Magistrato A.*, Robertazzi A., Carloni P. **'**Nitrogen Fixation by a Molybdenum Catalyst Mimicking the Function of the Nitrogenase Enzyme: A Critical Evaluation of DFT and Solvent Effects' *J. Chem. Theor. Comput.* (2007) *3,* 1708-1720

Simona F., Magistrato A., Vera D.M., Garau G., Vila A. J., Carloni P. 'Protonation State and Substrate Binding to B2 Metallo-beta-Lactamase CphA from Aeromonas Hydrofila' *Proteins.* (2007) 69, 595-605

Corral E., Hotze A.C.G., Magistrato A., Reedijk J. 'Interaction between the DNA Model Base 9-ethylguanine and a Group of Ruthenium Polypyridyl Complexes: Kinetics and Conformational Temperature Dependence' *Inorg. Chem.* (2007) 46, 6715-6722

Robertazzi A., Magistrato A.*, de Hoog P., Carloni P., Reedijk J. 'Density Functional Theory Studies on Copper Phenanthroline Complexes' *Inorg. Chem*, (2007) 46, 5873-5881

Magistrato A.*, Ruggerone P., Spiegel K., Carloni, P., Reedijk J. 'Binding of Novel Azole-Bridged Dinuclear Platinum(II) Anticancer Drugs to DNA. Insights from QM/MM Molecular Dynamics Simulations' *J. Chem. Phys. B* (2006) 110, 3604-3613

Vargiu A., Ruggerone P., Magistrato A., Carloni P. 'Molecular Recognition of DNA by Minor Groove Binders. Insights from Molecular Dynamics Investigation of the Interaction between Anthramycin and DNA' *J. Phys. Chem. B* (2006) 110, 24687-24695

Cascella M., Magistrato A., Tavernelli I., Carloni P., Rothlisberger U. 'Role of Protein Frame and Solvent for the Redox Properties of Azurin from Pseudomonas Aeruginosa' *Proc. Natl. Acad. Sci. USA* (2006) 103, 19641-19646

Spiegel K., Magistrato A.* 'Modeling Anticancer Drug-DNA Interactions from Mixed QM/MM Molecular Dynamics Simulations' *Org. Biomol. Chem* (2006) 4, 2507-2517

Magistrato A.*, Woo T.K., Togni A., Rothlisberger U. 'Enantioselective Palladium Catalyzed Hydrosilylation of Styrene: Influence of Electronic and Steric Effects on Enantioselectivity and Catalyst Design via Hybrid QM/MM Molecular Dynamics' *Organometallics*, (2006) *25*, 1151-1157

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Book Chapters

Rossetti G and Magistrato A.* Molecular Mechanism of Huntington's Disease: A computational Perpesective. In Huntington's Disease- Core Concepts and Current Advances Edited by N.E. Tunali ISBN 978-953-307-953-0 Chapter 3 (invited chapter)

Robertazzi A., Magistrato A, Dal Peraro M, Carloni P. (2010) First Principles DFT Studies of Metal-Based Biological and Biomimetic Systems in Metallic Systems: A Quantum Chemists's Perspective, Chapter 1. Edited by Carlos A . Gonzalez CRC Press 2011 Print ISBN: 978-1-4200-6077-5 eBook ISBN: 978-1-4200-6086-7, DOI: 10.1201/b10835-2 (invited chapter)

Magistrato A., Carloni P. (2005) 'Ab initio Molecular Dynamics Simulations of Biological Relevant Systems' *Handbook of Material Modeling,* vol 1, 259-274 (invited chapter)

Magistrato A., Togni A., Rothlisberger U., Woo T.K. (2002), 'Molecular Modeling of Enantioselective Hydrosilylation by Chiral Pd Based Homogeneous Catalysts with First-Principles and Hybrid QM/MM Molecular Dynamics Simulations' *Computational Modelling of Homogeneous Catalysis*, Maseras F, Lledos A (Eds.), Kluwer Academic, Dordrecht (the Netherlands). p 213-252. (invited chapter)

Organizational Experience

July 2018 Paris France CECAM workshop 'Frontiers and challenges of computing metals for biochemical, medical and technological applications' Alessandra Magistrato, Marco De Vivo, Gianluca Lattanzi, Carlo Adamo, Giulia Palermo, Ursula Roethlisberger

June 2017, CECAM School for Atomistic Simulations Trieste Organized by A. Magistrato, S. DeGironcoli, A. Dal Corso.

May 2016, CECAM meeting 'Structural and Functional Annotation of Bioinorganic Systems: Perspectives and Challenges from Theory and Experiments' Pisa 2016 Organized by A. Magistrato, P. Carloni, G. Legname, R. Nechustai, G. Brancato, V. Barone.

December 2009, Psi-K, SimBioMa, CECAM meeting 'Ab initio Modeling In Applied Biosciences, Structure, Dynamics and Function', December 11-12th Uppsala, Sweden. Organized by P. M. Panchmatia, B. Sanyal, P. M. Oppeneer, O. Eriksson, Uppsala University, Sweden, A. Magistrato and P. Carloni SISSA and CNR-INFM-Democritos, Trieste, Italy.

May 2004, psi-k Symposium on 'Ab initio Modeling of Biological Systems', Trieste, Italy. Organized by A. Magistrato, S. Raugei, P. Carloni