Curriculum Vitae

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.

Career

June 2006 –present	Permanent position as research associate at CNR-IOM-Democritos National Simulation Center hosted by the International School for Advanced Studies (SISSA), Trieste, Italy.
Jan 2003 – June 2006	Tenure Track fellow 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).

Leaves Periods

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

Fellowships

Postdoctoral fellowship of the Swiss National Foundation July 2001-July 2002 hosted in the group of Prof. M.L. Klein, University of Pennsylvania, Philadelphia, PA, USA.

Pubblications

Author of 62 articles, 4 book chapters, 8 Conference Proceedings

H-index: 24 (font Google Scholar, July 2016) Citations: 1494

Awards

2013 Abilitation as Associate Professor in Theoretical Physics of Matter
2013 Abilitation as Associate Professor in Chemistry and Inorganic Chemistry
Award for the best oral presentation at the Fall Meeting of the Swiss Chemical Society, Basel-CH (2000)
Award for the best poster presentation at the INFM-Meeting, Genova, Italy, 2004

Supervision Experience

2004-2015 supervisor of
9 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-, SISSA), Maria Letizia Merlini (EPFL, Lausanne) .

6 postdocs: Aneta Jezierska (2008), Arturo Robertazzi (2006-2008), Branimir Bertosa (2008-2009), Jacopo Sgrignani (2010-2012), Angelo Spinello (2016-), Matic Pavlin (2016-);

2 bachelor students: Marta Bon (February-November 2013), Nadira Abdurakhmanova (2013-2015).

Peer Reviewer Activity

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

Funding Agencies

Swiss National Science Foundation, National Science Foundation, USA, CNR-INFM, Croatian Science Foundation, PRACE Infrastructure, Italian-French University, Austrian Science Foundation, French National Science Foundation, Dutch National Science Fundation.

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).

Organizational Experience

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.

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

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.

Grants

PI of 'My first airc grant' (220000 €) financed by AIRC 2016-2018

Participant to the 'Nanoscience Fiundries and Fine Analysis' Founded by Horizon 2020 (2015-2019) (2758161 €).

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

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)

Co-PI of the 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)

PI of 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).

Co-PI of 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)

Co-PI of 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)

Co-PI of two grants for PhD students given by the Italian Minister of Education for 'Theoretical Investigations of Drug/Target interactions' (€ 60,000)

Grants for Computing

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).

Teaching Experience

2014-2015 Lectures on 'Simulation in molecular medicines'

2011 Lectures on 'Simulation in molecular medicines' and 'Principles of Quantum Chemistry'.

2003-2008 annual series of lectures and exercises in 'Principles of Quantum Chemistry'.

2001 and 2000 October-March Assistantship position for the Inorganic Chemistry Laboratory for the undergraduate students of pharmacy at the ETH Zentrum, Zürich, Switzerland.

January 2000 Lectures in theoretical inorganic chemistry at 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 at Conferences

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

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

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

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

AIMECS 2007, Istanbul, Turkey, July 11st 2007

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

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

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

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

Invited Talks at international Institutions

University of Calabria, Cosenza IT December 10th 2015

Juelich Forchungzentrum July 2nd 2015

Institute for research in Biomedicine, Bellinzona, CH April 2015

University of Namur, Belgium, January 20th 2015,

University of Wien BOKU, October 9th 2014

EPFL, Lausanne, Switzerland, February 14th 2014

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

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

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

SIGEA Meeting, Milan, November, 14th, 2006

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

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

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 Publication

L Casalino, G Palermo, U Rothlisberger, A Magistrato Who Activates the Nucleophile in Ribozyme Catalysis? An Answer from the Splicing Mechanism of Group II Introns Journal of the American Chemical Society (2016)

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

L. M. R. Napolitano, I. Bisha, M. De March, A. Marchesi, M. Arcangeletti, N. Demitri, M. Mazzolini, A. Rodriguez, A. Magistrato, S. Onesti, A. Laio,V. Torre 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

J Sgrignani, A Magistrato 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), pp 3864–3875

I Bisha, A Rodriguez, A Laio, A Magistrato 'Metadynamics Simulations Reveal a Na+ Independent Exiting Path of Galactose for the Inward-Facing Conformation of vSGLT' PLoS computational biology 10 (12), e1004017 (2014)

J Sgrignani, M Bon, G Colombo, A Magistrato 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 A. V.; Magistrato A. (2014) 'The dissociation of metallo-intercalators from DNA is tuned by their shape and charge' 53 (15), 7999-8008

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

Franco, D.; Sgrignani, J.; Bussi, G.; Magistrato A (2013) 'The Structural Role of Uracil DNA Glycosylase for the Recognition of Uracil in DNA duplexes. Clues from Atomistic Simulations' *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 (2013) 'Functionalized Fe-Filled Multiwalled Carbon Nanotubes as Multifunctional Scaffolds for Magnetization of Cancer Cells' *Adv. Funct. Mat.* 23 (25), 3173-3184 (Cover Picture).

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

Sgrignani J., Magistrato A. (2012) '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.* 52 (6), 1595-1606 (Cover Image).

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

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

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

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. (2010) 'Bioinorganic Chemistry of Parkinson's Disease: Structural Determinants for the Copper-Mediated Amyloid Formation of Alpha-Synuclein' *Inorg. Chem.* 49, 22, 10668-10679.

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

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

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

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

Brancia F.L., Stener M., Magistrato A. (2009) '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.* 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. (2009) 'Synthesis, Photophysical, and Electrochemiluminescent Properties of 5,15-Bis(9-antracenyl)porphyrins Derivatives' Org. Biomol. Chem., 7, 11, 2402-2413

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

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

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

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

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

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

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

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

Magistrato A., Robertazzi A., Carloni P. (2007) **'**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. 3,* 1708-1720

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

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

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

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

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

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

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

Maurer P., Magistrato A., Rothlisberger U. (2004) 'Theoretical Studies of C-S Bond Cleavage in Complexes of the Form $[M(9S3)_2]^{2+}$ (M=Re,Tc, Ru and 9S3=trithiaciclononane)' *J. Phys. Chem. A* 108, 11494-11499 (2004).

Krumper J. R., Gerisch M., Magistrato A., Rothlisberger U., Bergman R. G., Don Tilley T. 'h1-Arene Complexes of Rhodium(III): Experimental Evidence and Theoretical Studies' (2005) *J. Am. Chem. Soc.* 126, 12492- 12502

Magistrato A., Woo T.K., Togni A., Rothlisberger U. (2004) 'Enantioselective Palladium-Catalyzed Hydrosilylation of Styrene: Detailed Reaction Mechanism from First-Principles and Hybrid QM/MM Molecular Dynamics Simulations' *Organometallics*, 23, 3218-3227

Magistrato A., Maurer P., Fassler T., Rothlisberger U.(2004). 'First-Principles Simulations of C-S Bond Cleavage in Rhenium Thioether Complexes' *J. Phys. Chem. A*, 108, 2008-2013

Magistrato A., DeGrado W.F., Laio A., Rothlisberger U., VandeVondele J. Klein M. L. (2003) 'Characterization of the Dizinc Analogue of the Synthetic Diiron Protein DF1 Using ab initio and Hybrid Quantum/Classical Molecular Dynamics Simulations' *J. Phys. Chem. B*, 107, 4182-4188

Macchioni A., Magistrato A., Orabona I., Ruffo F., Rothlisberger U., Zuccaccia C. '(2003) Direct Observation of an Equilibrium Between Two Anion-Cation Orientations in Olefin Pt(II) Complex Ion Pairs by HOESY NMR Spectroscopy' *New J. Chem.*, 27, 455-458 .

Dotta P., Magistrato A., Rothlisberger U., Pregosin P.S., Albinati A. (2002) 'Dialkyl Effect on Enantioselectivity: p-stacking as a Structural Feature in P,N Complexes of Palladium(II)' *Organometallics*, 21, 3033-3041

VandeVondele J., Magistrato A., Rothlisberger U. (2001) 'Cis-Trans Isomerization in Triply-Bonded Ditungsten Complexes: A Multitude of Possible Pathways' *Inorg. Chem.*, 40, 5780-5786

Magistrato A., Pregosin P.S., Albinati A., Rothlisberger U. (2001) 'The Role of p-p Stacking Interactions in Square Planar Palladium Complexes. Combined Quantum Mechanics/Molecular Mechanics QM/MM Studies' *Organometallics*, 20, 4178-4184

Loss S., Magistrato A., Cataldo L., Hoffmann S., Geoffroy M., Rothlisberger U., Grutzmacher H. (2001) 'Isolation of a Highly Persistent Diphosphanyl Radical: The Phosphorus Analogue of a Hydrazyl' *Angew. Chem. Int. Edit.*, 40, 723-726

Magistrato A., VandeVondele J., Rothlisberger U. (2000) 'Three- and Four-center Trans Effects in Triply Bonded Ditungsten Complexes: An ab initio Molecular Dynamics Study of Compounds with Stoichiometry $W_2Cl_4(NHEt)_{(2)}(PMe_3)_{(2)}$' *Inorg. Chem.*, 39, 5553-5560

Magistrato A., Merlin M., Pregosin P.S., Rothlisberger U., Albinati A. (2000) 'Electronically and Sterically Induced Structural Distortions in Square-Planar d(8) Complexes' *Organometallics*, 19, 3591-3596

Peer Reviewed Reviews

J Sgrignani, A Cavalli, G Colombo, A Magistrato
Enzymatic and Inhibition Mechanism of Human Aromatase (CYP19A1) Enzyme. A Computational Perspective from QM/MM and Classical Molecular Dynamics Simulations. Mini reviews in medicinal chemistry (2016)

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

G Palermo, A Magistrato, T Riedel, T Von Erlach, CA Davey, PJ Dyson, ...
Fighting Cancer with Transition Metal Complexes: From Naked DNA to Protein and Chromatin Targeting Strategies ChemMedChem 2015

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

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

Vargiu A.V. and 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 9 (9), 1966-1981

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

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

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

Colombo M.C., Guidoni L., Laio A., Magistrato A., Maurer P., Piana S., Rohrig U., Spiegel K., Sulpizi M., VandeVondele J., Zumstein M., Rothlisberger U. (2002) 'Hybrid QM/MM Car-Parrinello Simulations of Catalytic and Enzymatic Reactions' *Chimia*, 56, 13-19

Book Chapters

1 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)

2 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)

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

4 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)