

# Curriculum vitae

## PERSONAL INFORMATION

Family name: MORANTE                      First name: SILVIA  
Nationality: Italian  
Date of birth: January 12th, 1954  
Personal web site URL:            <http://biophys.roma2.infn.it/index.php/group-members/50-morante-web-page>  
Group web site URL:                <http://biophys.roma2.infn.it>

## • EDUCATION

1977            Master (Laurea) in Physics *magna cum laude* - Department of Physics, University of Rome, La Sapienza, Rome, Italy

## • CURRENT POSITION

2012 - today    Full Professor - Department of Physics, University of Rome Tor Vergata, Roma, Italy  
2007 - today    Associate Researcher - Group IV (Theoretical Physics) INFN - Tor Vergata, Roma, Italy  
2012 - today    Associate Researcher - ICCOM - CNR - Area Ricerca CNR, Firenze, Italy  
2004 - today    Associate Researcher - CAST (Centro interdipartimentale per il Calcolo Avanzato nella Scienza e nella Tecnica), University of Rome Tor Vergata, Roma, Italy

## • PREVIOUS POSITIONS

2000 - 2012    Associate Professor    Department of Physics, University of Rome, Tor Vergata, Roma, Italy  
2000 - 2007    Associate Researcher    Group V (Technological Research) INFN - Tor Vergata, Roma, Italy  
1984 - 2000    Assistant Professor    Department of Physics, University of Rome, Tor Vergata, Roma, Italy  
1980 - 1984    Assistant Professor    Department of Physics, Free University of Trento, Trento, Italy  
1978 -1979    Research Fellow        Istituto Trentino di Cultura, Trento, Italy  
1977 -1978    Research Fellow        Department of Physics, University of Trento, Trento, Italy

## • SUPERVISION OF GRADUATE, MASTER AND DOCTORAL THESIS

1989 - today    24 Master thesis, 9 Graduate Thesis and 8 Doctoral Thesis

## • TEACHING ACTIVITIES

1984 - today    Member of tens of PhD thesis Committees  
2007 - today    Professor - Biophysics e-Master in “Frontiere della Fisica”, University of Rome, Tor Vergata, Roma, Italy  
2005 - today    Professor - Biophysics e-Master in “Nature, Science, Epistemology and Pedagogy”, University of Rome, Tor Vergata, Roma, Italy  
2002 - today    Professor - Advanced Biophysics - Department of Physics, University of Rome, Tor Vergata, Roma, Italy  
1991 - today    Professor - Introductory Biophysics, Department of Physics, University of Rome, Tor

Vergata, Roma, Italy

1997 - 2011 Professor - Biophysics for PhD students in Physics - Department of Physics, University of Rome, Tor Vergata, Roma, Italy

2004 - 2005 Professor - Biophysics School for PhD students in Physics - Department of Biophysics - Humboldt University, Berlin, Germany

2001-2002 Professor - Biophysics School for PhD students in Physics - Department of Biophysics - Humboldt University, Berlin, Germany

1998 - 1999 Professor - Biophysics for PhD students in Physics - Department of Biophysics - Humboldt University, Berlin, Germany

1992 - 1995 Professor - Laboratory Course - Scienze Ambientali Università della Tuscia, Viterbo, Italy

• **VISITING SCIENTIST**

1999 Humboldt University - Insitute for Theoretical Biophysics (Berlino - Germany)

2000 - 2001 ESRF (Grenoble - France)

2005 Humboldt University - Insitute for Theoretical Biophysics (Berlino - Germany)

2006 - 2010 A few months spent between Humboldt University - Insitute for Theoretical Biophysics (Berlino - Germany) and NIC - DESY Zeuthen (Zeuthen, Germany)

• **ORGANISATION OF SCIENTIFIC MEETINGS**

1984 - today Chairperson / Scientific Committee member / Organizing Committee member of numerous (about 25) international and national conferences

• **INSTITUTIONAL RESPONSIBILITIES**

1984 - today Head of the Biophysics Research Group Department of Physics, University of Rome, Tor Vergata, Roma, Italy

2012 - 2016 Member of the executive committee of SIBPA (Società Italiana di Biofisica Pura e Applicata)

2011 - 2017 Member of the executive committee of C6 (Biological Physics) of IUPAP (International Union of Pure and Applied Physics)

2012 - today IUPAP representative for the connectivity with IUPAB (International Union of Pure and Applied Biophysics)

2008 - 2012 National Representative at EBSA (European Biophysical Societies' Association)

2008 - 2012 President of SIBPA (Società Italiana di Biofisica Pura e Applicata)

2004 - 2008 Member of the executive committee of SIBPA (Società Italiana di Biofisica Pura e Applicata)

2015 – 2020 Member of the Review Committees at ESRF

• **COMMISSIONS OF TRUST**

1. Scientific Evaluator for “FWO’s 2019 Call for Junior and Senior Research Projects”
2. Scientific Evaluator for “Agence National de la Recherche” (ANR), France
3. Expert evaluator for Marie Curie post doc fellowship
4. Member of numerous national fellowship and assistant research evaluation Committees
5. Member of the Editorial Board:
  - Dataset Papers in Biophysics
  - Theoretical Biology Forum
5. Referee for the following scientific journal

*Journal of Physical Chemistry*  
*Journal of European Biophysical Journal*  
*Journal of Theoretical Biology*  
*Langmuir*  
*Journal of Inorganic Chemistry*  
*Computational Biology Journal*  
*Journal of Inorganic Biochemistry*  
*Metallomics*  
*ACS Chemical Neuroscience*  
*Physical Chemistry Chemical Physics*  
*PLoS Computational Biology*  
*Theoretical Biology Forum*  
*Journal of Physical Chemistry*  
*Nature Chemical Biology*  
*Computational Biology and Chemistry*

- **MEMBERSHIPS OF SCIENTIFIC SOCIETIES**

Member of EBSA (European Biophysical Societies' Association)  
Member of SIBPA (Società Italiana di Biofisica Pura e Applicata)  
Member of SIF (Società Italiana di Fisica)

- **INVITED and PRESENTED TALK**

1977 - today: About 80 invited talks in International Conferences  
1977 - today: About 100 talks/posters presented in International and National Conferences

2009 Spokesperson of the BioFEL Collaboration in “FEL’s light into life: The value of SPARX for life sciences”

2017 (1-12) - Bari  
2018 – Erice  
2018 - Rostov

- **SCIENTIFIC PRODUCTS**

**Publications (see attached Publication list)**

Author of about 90 research papers: 69 Peer reviewed publications in international journals and invited reviews; 11 Peer Reviewed Paper in Conference Proceedings; 11 Invited reviews and book’s chapters

**Patents**

Granted of the international patent: “Preparation procedure of vaccines based on the identification of amino acidic sequences of the HIV antigens similar to host protein sequences”. Patent ID RM 92 A 000157. Date 06/March/1992, international class: A 61 K.

- **CURRENT MAJOR INTERNATIONAL COLLABORATIONS**

O. Proux, ESRF, Grenoble (FR)

H. Chapman, Center for Free Electron Laser Science, DESY, Hamburg (DE)  
G. Millhauser, Department of Chemistry University of California, Santa Cruz (USA)  
S. Saxena, Department of Chemistry, Chevron Science Center, Pittsburgh (USA)  
M. Calandra, Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie  
Université Pierre et Marie Curie, Paris (FR)  
C. Exley, Keele University, UK  
F. Dacapito, CNR-IOM-OGG, ESRF, Grenoble (FR)

- **CURRENT MAJOR NATIONAL COLLABORATIONS**

V. Consalvi, Department of Biochemistry University of Rome La Sapienza, Roma, (IT)  
G. La Penna, National Research Council (CNR), Institute for Chemistry of Organometallic  
Compounds, Sesto fiorentino (IT)

- **RESEARCH FUNDING**

**Approved and Granted**

- **PRIN 2019**

- **Moleti**

- 2015 – 2016, Uncovering Excellence (A. Filabozzi, P.I.): “*The goods and the bads of protein fibrillation*”
- 2013 - 2015 (national coordinator of Quantitative Biology section) - Progetto Premiale INFN SUMA
- 2000 - today (local coordinator) - Iniziativa Specifica INFN: TO61 and Biophys
- 2008 - 2010, MIUR, PRIN08 (local coordinator)
- 2005 - 2007, MIUR, PRIN05 (local coordinator)
- 1984 - 2005, Research funded by the following national agencies: CNR (GNCB, Comitato Biotecnologie, Comitato Fisica); MURST (40%, 60%, COFIN); INFM (Sezione B); INFN (gruppo V); MIUR

- **BEAM TIME ALLOCATION IN INTERNATIONAL X-RAY FACILITIES**

- **Mettere le ultime**

- 2014-2015 ESRF (2014) (P.I.) - “*A study on how Zn(II) ions perturb Cu(II) coordination to A-beta peptides and modulate the peptide aggregation thus possibly affecting the Alzheimer disease progression*”
- 2010 ESRF (P.I.): “*Copper binding effect on Zinc coordination mode of synthetic peptides mimicking Prion Protein sequence*”
- 2009 ESRF (P.I.): “*Zinc binding effect on Copper coordination mode of synthetic peptides mimicking Prion Protein sequence*”

- **COMPUTER TIME ALLOCATION IN EUROPEAN COMPUTING CENTERS**

- **Mettere gli altri al CINECA**

- 2011 - 2012 NIC (John von Neumann-Institut für Computing) “*The role of metals in beta-amyloid interactions. A proposal for an ab initio study*”, 50.000 core/hours at JUROPA (PC cluster, IBM Power4)
- 2010 NIC (John von Neumann-Institut für Computing): “*The role of metals in beta-amyloid interactions. A proposal for an ab initio study*”, 100.000 core/hours at the Supercomputer JUGENE (IBM BlueGene/P), Juelicher Supercomputer Center (JSC)
- 2009 DEISA Extreme Computing Initiative (Seventh Framework Programme 2009): “*The rôle of metals in beta-amyloid interactions. A proposal for an ab initio study*”, 400.000 core/hours at the Cray XT4 Supercomputer (Louhi, Finland)

## • CURRENT SCIENTIFIC ACTIVITY

Proteins are essential for almost every cellular activity. Their conformational heterogeneity and their ability to visit huge numbers of free energy minima (conformational substates) are the key properties for the understanding of their surprising versatility. While residing in a given structural conformation, they still exhibit a broad spectrum of motions, from local fluctuations of single atoms to structural rearrangements of large extension, with characteristic time spans from picoseconds to minutes. The substates population and the interconversion kinetics among different substates are influenced by the presence of cofactors like, in particular, transition metal ions.

The recent spectacular improvement achieved in X-ray sources brilliance and the increase in the computing performances of parallel supercomputers make today possible to attack structural problems of the highest biological importance that have until now largely defeated the efforts of the scientific community. Among them understanding the phenomenon of protein aggregation is becoming more and more urgent because of its relevance in a vast area of biological researches and applications, ranging from the study of amyloid diseases to the need of better controlling industrial processes like drug synthesis and food preservation.

At the moment the Tor Vergata Biophysics group is strongly focused on the study of the phenomenon of protein aggregation in the presence of metals dwelling on a synergic use of quantum-mechanical simulations to understand the recently available synchrotron- and Free Electron Laser-based XAS and XRD data.

Indeed, it is generally believed that metals play an important role in the misfolding and aggregation phenomena that lead to the development of neurodegenerative diseases like the Alzheimer's disease (AD) and prion diseases. Metal ions have been found in complex with both  $\beta$ -amyloid ( $A\beta$ ) peptides and Prion Protein (PrP) that are the main proteinaceous components of the amyloid brain deposition detected in patients.

Relying on a combination of classical molecular dynamics (MD) and hybrid QM/MM computational methods, we have recently studied the influence of the nature of the local physico-chemical environment on the structural features of  $\beta$ -amyloid peptides complexed with Zn(II) ions. The analysis is carried out by comparing among themselves different Zn(II)-ligand force fields and studying their influence on metal coordination and long-range peptide folding. The system in the non-physiological so-called “gas phase” (no solvent) was also simulated with the purpose of identifying to what extent, if at all, the solvent can affect the Zn

coordination mode, besides its long-range structural properties. There are two main results of this investigation: i) the Zn(II) coordination mode in classical MD simulations is found to markedly depend on the partial charge attributed to the ion and the atoms surrounding it. In this investigation we have been able to identify the most appropriate Zn(II) force field for the Zn(II)–A $\beta_{1-16}$  complex; ii) although the presence of water obviously influences the peptide folding propensity, it does not affect the structure of the Zn(II) inner coordination shell. Classical results are validated using a hybrid QM/MM optimization step.

XAS measurements have been carried out also on various portions of Prion-protein tetra-octarepeat peptides in complexes with Cu(II) ions, both in the presence and in the absence of Zn(II). Because of the ability of the XAS technique to provide detailed local structural information, we demonstrated that Zn (by directly interacting with the peptide) competes with Cu for peptide binding and viceversa. This finding suggests that metal binding competition can be important in the more general context of metal homeostasis.

With the aim of finding anti-aggregation oligopeptides with therapeutic effect, we have used extensive molecular dynamics simulations of model systems comprising an A $\beta_{1-40}$  peptide in water in interaction with short peptides ( $\beta$ -sheet breakers) mimicking the 17–21 region of the A $\beta_{1-40}$  sequence. Various systems differing in the customized  $\beta$ -sheet breaker structure have been studied. Simulation results confirm experimental data (thioflavin T fluorescence, circular dichroism, and mass spectrometry), indicating that  $\beta$ -sheet breakers are able to inhibit in vitro fibril formation and prevent the  $\beta$ -sheet folding of portions of the A $\beta_{1-40}$  peptide. Furthermore far UV circular dichroism experiments suggested by molecular dynamics simulations have provided consistent evidence that a newly devised Ac-LPFFN-NH<sub>2</sub>  $\beta$ -sheet breaker is more effective than those known in the literature in stabilizing the native  $\alpha$ -helix structure of A $\beta_{1-40}$ . In agreement with these findings thioflavin T fluorescence experiments also confirmed its higher efficiency in inhibiting A $\beta_{1-40}$  aggregation. Furthermore, mass spectrometry data and molecular dynamics simulations consistently identified the 17–21 A $\beta_{1-40}$  portion as the location of the interaction region between A $\beta_{1-40}$  peptide and the Ac-LPFFN-NH<sub>2</sub>  $\beta$ -sheet breaker.

Parallel to this activity we have been trying to theoretically attack one of the major challenges in biology, namely the problem of understanding how molecular processes determine phenotypic features. We addressed this fundamental problem in a class of model systems designed to describe the dynamics of channel activity by developing a general mathematical framework that allows the calculation of mesoscopic properties from the knowledge of microscopic description of the elementary degrees of freedom of the system. We demonstrated how experimentally accessible quantities, such as opening and closing times and the coefficient of variation of inter-spike intervals, and other, more elaborated, quantities can be analytically calculated from the underlying microscopic Markovian dynamics. We emphasize that our formulae fully agree with results obtained by stochastic simulations and approaches based on a full determination of the microscopic system's time evolution. We also illustrate how experiments can be devised to discriminate between alternative molecular models of the inositol-trisphosphate receptor. The developed approach is applicable to any system described by an underlying Markov process and, owing to the analytic nature of the resulting formulae, provides an easy way to characterize also rare events that are of particular importance to understand the intermittency properties of complex dynamic systems.

From a more experimental point of view we are engaged in a collaboration with one of the leading group in the exploitation of FEL radiation in Biophysics, with the aim of developing new methodologies (in particular in serial crystallography), instrumentation (optic to focus pulses of 4.3 nm photons from the Hamburg Free-Electron Laser at normal incidence) and technology (in vivo crystallization) for FEL experiments on systems of biological interest.

## List of publications

**Silvia Morante**

### Peer reviewed publications in international journals and invited reviews

1. F. Stellato, R. Chiaraluce, V. Consalvi, E. De Santis, G. La Penna, O. Proux, G. Rossi and S. Morante “Dealing with Cu reduction in X-ray Absorption Spectroscopy experiments” *Metallomics*, 2019, DOI: 10.1039/C9MT00110G
2. L. Serafini, A. Bacci, A. Bellandi et al., “MariX, an advanced MHz-class repetition rate X-ray source for linear regime time-resolved spectroscopy and photon scattering.” *Nuclear Inst. and Methods in Physics Research, A* (2019), <https://doi.org/10.1016/j.nima.2019.03.096>
3. E. De Santis, E. Shardlow, F. Stellato, O. Proux, G. Rossi, C. Exley and S. Morante, “X-Ray Absorption Spectroscopy Measurements of Cu-ProIAPP Complexes at Physiological Concentrations” (2019) *Condens Matter*. 4(1): 13.
4. F. Villa, A. Cianchi, M. Coreno, S. Dabagov, A. Marcelli, V. Minicozzi, S. Morante, F. Stellato. (2018) “Design study of a photon beamline for a soft X-ray driven by high gradient acceleration at EuPRAXIA@SPARC\_LAB” *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*. **909**: 294-297.
5. F. Stellato, M. Calandra, F. D’Acapito, E. De Santis, G. La Penna, G. Rossi, and S. Morante, “Multi-scale theoretical approach to X-ray absorption spectra in disordered systems: an application to the study of Zn(II) in water” (2018) *PCCP* submitted
6. M Ferrario et al., “EuPRAXIA@SPARC\_LAB Design study towards a compact FEL facility at LNF” (2018). <https://doi.org/10.1016/j.nima.2018.01.094>

7. M. Carbonaro, F. Ripanti, V. Minicozzi, F. Stellato, E. Placidi, S. Morante, A. Di Venere, E. Nicolai, P. Postorino, A. Nucara, "Human insulin fibrillogenesis in the presence of epigallocatechin gallate and melatonin: structural insights from a biophysical approach." (2018) *International Journal of Biological Macromolecules* 10.1016/j.ijbiomac.2018.04.13
8. E. Capozzi, V. Minicozzi, S. Aureli, G.C. Rossi, F. Stellato, and S. Morante "Designing effective anticancer-radiopeptides. A Molecular Dynamics study of their interaction with model tumor and healthy cell membranes. (2018) *BBA Biomembranes* <https://doi.org/10.1016/j.bbamem.2018.05.021>
9. F. Stellato, Z. Fusco, R. Chiaraluce, V. Consalvi, S. Dinarelli, E. Placidi M. Petrosino, G. C Rossi, V. Minicozzi, S. Morante, "The effect of  $\beta$ -sheet breaker peptides on metal associated Amyloid- $\beta$  peptide aggregation process" (2017) *Biophysical Chemistry*, **229** 110-114. doi: 10.1016/j.bpc.2017.05.005
10. S. Morante and G.C. Rossi, "From the Scientific Optimism of the Age of Enlightenment to the Problems of Modern research Conceptualization" (2017) *Giornale di Fisica*, **58:1**
11. M. Petrosino, L. Lori, A. Pasquo, C. Lori, V. Consalvi, V. Minicozzi, S. Morante, A. Laghezza, A. Giorgi, D. Capelli, R. Chiaraluce, "Single Nucleotide Polymorphism of PPAR Gamma, A protein at the crossroads of physiological and pathological processes." (2017) *International Journal of Molecular Science* 18:361; doi:10.3390/ijms18020361
12. S. Morante and G.C. Rossi, "A novel proof of the DFT formula for the interatomic force field of Molecular Dynamics" (2017) *Annals of Physics Annals* **37**: 71–76
13. M. Carbonaro, A. Di Venere, A. Filabozzi, P. Maselli, V. Minicozzi, S. Morante, E. Nicolai, A. Nucara, E. Placidi, F. Stellato "Role of dietary antioxidant (-)-epicatechin in the development of b-lactoglobulin fibrils" (2016) *BBA - Proteins and Proteomics* 1864: 766-772 DOI: 10.1016/j.bbapap.2016.03.017
14. E. De Santis, V. Minicozzi, S. Morante, G.C. Rossi, F. Stellato "The role of metals in protein conformational disorders – The case of prion protein and A $\beta$ -peptide" (2016) *Journal of Physics: Conference Series* **689**: 012028
15. S. Morante and G.C. Rossi, "The notion of scientific knowledge in biology" (2016) *Science & Education*, **25**(1-2) 165-197. DOI:10.1007/s11191-015-9803-5
16. F. Stellato, Z. Fusco, R. Chiaraluce, V. Consalvi, S. Dinarelli, S. Morante, M. Petrosino, G. C Rossi, "The effect of  $\beta$ -sheet breakers peptides on metal associated Amyloid- $\beta$  peptide aggregation process" (2016) *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* submitted
17. M. Carbonaro, A. Di Venere, A. Filabozzi, P. Maselli, V. Minicozzi, S. Morante, E. Nicolai, A. Nucara, E. Placidi, F. Stellato "Role of dietary antioxidant (-)-epicatechin in the development of b-lactoglobulin fibrils" (2016) *BBA - Proteins and Proteomics* 1864: 766-772 DOI: 10.1016/j.bbapap.2016.03.017

18. E. De Santis, V. Minicozzi, S. Morante, G. C. Rossi, F. Stellato “The role of metals in protein conformational disorders - The case of prion protein and A $\beta$ -peptide” (2016) *Journal of Physics: Conference Series* **689**: 012028E. De Santis, V. Minicozzi, S. Morante, G. C. Rossi, F. Stellato “The role of metals in Protein conformational disorders - The case of prion and  $\beta$ -Amyloid” (2016) *J Phys Chem B. 2015 Dec 31;119(52):15813-20*. doi: [10.1021/acs.jpcc.5b10264](https://doi.org/10.1021/acs.jpcc.5b10264).
19. S. Morante and G. C. Rossi, “The notion of scientific knowledge in biology” (2016) *Science & Education*, DOI:10.1007/s11191-015-9803-5
20. E. De Santis, V. Minicozzi, S. Morante, O. Proux, G. C. Rossi, S. Saxena, K. I. Silva, F. Stellato “Cu(II)-Zn(II) cross-modulation in amyloid-beta peptide binding: an X-ray Absorption Spectroscopy study” (2015) *J. Phys. Chem. B.* **119**, 15813–15820  
doi: [10.1021/acs.jpcc.5b10264](https://doi.org/10.1021/acs.jpcc.5b10264)
21. G. La Penna, V. Minicozzi, S. Morante, G. C. Rossi, F. Stellato “A first-principles calculation of the XANES spectrum of Cu<sup>2+</sup> in water” (2015) *Journal of Chemical Physics*, **143**, 124508 (2015); doi: [10.1063/1.4931808](https://doi.org/10.1063/1.4931808)
22. M. G. Di Carlo, V. Minicozzi, V. Foderà, V. Militello, V. Vetri, S. Morante, and M. Leone, “Thioflavin T controls A $\beta$ (1-40) peptide conformation and templates its aggregation pathway.” (2015) *Biophysical Chemistry* **206**:1-11.  
doi: [10.1016/j.bpc.2015.06.006](https://doi.org/10.1016/j.bpc.2015.06.006)
23. F. Stellato, V. Minicozzi, G. L. Millhauser, M. Pascucci, O. Proux, G. C. Rossi, A. Spevacek, S. Morante, “Copper–Zinc cross-modulation in prion protein binding.” *European Biophysical Journal* (2014) **43**: 631-642.
24. S. Morante, G. C. Rossi “Metals in Alzheimer’s Disease: A Combined Experimental and Numerical Approach” in *Advances in Alzheimer’s Research Volume 2*: 100-147 DOI: [10.2174/97816080585251140201](https://doi.org/10.2174/97816080585251140201)  
eISBN: 978-1-60805-852-5, 2014 ISBN: 978-1-60805-853-2 ISSN: 2214-4358.
25. V. Minicozzi, R. Chiaraluce, V. Consalvi, C. Giordano, C. Narcisi, P. Punzi, G. C. Rossi and S. Morante, “Computational and experimental casus on beta sheet breakers targeting A $\beta$ <sub>1-40</sub> fibrils.” *J. Biol. Chem.* (2014) **289**, 11242-11252. doi: [10.1074/jbc.M113.537472](https://doi.org/10.1074/jbc.M113.537472)
26. N. Christian, A. S. Skupin, S. Morante, K. Jansen, G. Rossi, O. Ebenhoeh “Mesoscopic behaviour from microscopic Markov dynamics and its application to calcium release channels” *J. Theor. Biol.* (2014) **343**, 102–112.
27. D. Alesini, M. Alessandrini, M. P. Anania, S. Andreas, M. Angelone, A. Arcovito, F. Arnesano, M. Artioli et al. “IRIDE White Book, An Interdisciplinary Research Infrastructure based on Dual Electron linacs&lasers” (2014) *Nucl.Instrum.Meth.* (2014) **A740**, 138-146 DOI: [10.1016/j.nima.2013.11.040](https://doi.org/10.1016/j.nima.2013.11.040)
28. A. Maiorana, T. Marino, V. Minicozzi, S. Morante, N. Russo. “A micro-environmental study of the Zn(II)-A $\beta$ 1-16 structural properties” *Biophysical*

*Chemistry* (2013) **182**, 86-93

29. R. Sarangi, P. Frank, M. Benfatto, S. Morante, V. Minicozzi, B. Hedman, K.O. Hodgson “The x-ray absorption spectroscopy model of solvation about sulfur in aqueous L-cysteine” *J. Chem. Phys.* **137**, 205103 (2012); doi: 10.1063/1.4767350
30. S. Morante, G.C. Rossi and M. Testa “The stress tensor of an atomistic system” **10**: 552-559 (2012) *Central European Journal of Physics* (CEJP) DOI:
31. P. Giannozzi, K. Jansen, G. La Penna, V. Minicozzi, S. Morante, G.C. Rossi, F. Stellato “Zn induced structural aggregation patterns of  $\beta$ -amyloid peptides by first-principle simulations and XAS measurements” *Metallomics*. **4(2)**:156-165 (2012). DOI: 10.1039/C2MT00148A
32. F. Stellato, A. Spevacek, O. Proux, V. Minicozzi, G. Millhauser, S. Morante “Zinc modulates Copper coordination mode in Prion Protein octa-repeat subdomains” *European Biophysical Journal* **40**: 1259-1270 (2011). DOI: 10.1007/s00249-011-0713-4
33. M. Salomone-Stagni, F. Stellato, C.M. Whaley, S. Vogt, S. Morante, S. Shima, T.B. Rauchfuss, W. Meyer-Klaucke “The iron-site structure of [Fe]-hydrogenase and model systems: an X-ray Absorption Near Edge Spectroscopy study” *Dalton Trans.* **39**: 3057-3064 (2010).
34. V. Minicozzi, S. Morante. “Is Cu involved in prion oligopeptide stability? Experiments and numerical simulations.” *International Journal of Quantum Chemistry* **110**: 656-680 (2010).
35. P.R. Crippa, M. Eisner, S. Morante, F. Stellato, F. C. Vicentin, L. Zecca. “A XAS Study of the Sulphur Environment in Human Neuromelanin and its Synthetic Analogues” *European Biophysical Journal*, **39(6)**: 959-70 (2010).
36. R. Besio, S. Alleva, A. Forlino, A. Lupi, C. Meneghini, V. Minicozzi, A. Profumo, F. Stellato, R. Tenni, S. Morante. “Identifying the structure of the active sites of human Prolidase.” *European Biophysical Journal*, **39(6)**: 935-45 (2010).
37. F. Guerrieri, V. Minicozzi, S. Morante, G. C. Rossi, S. Furlan, G. La Penna. “Modeling the interplay of glycine protonation and multiple histidine binding of copper in the Prion protein octarepeat sub-domains” *Journal of Biological Inorganic Chemistry*, **14**: 361-74 (2009).
38. V. Minicozzi, S. Morante, G.C. Rossi, F. Stellato, N. Christian, K. Jansen. “The role of metals in aggregation. Experiments and *ab initio* simulations” *International Journal of Quantum Chemistry*, **108**: 1992-2015 (2008).
39. V. Minicozzi, F. Stellato, M. Comai, M. Dalla Serra, C. Potrich, W. Meyer-Klaucke, S. Morante. “Identifying the Minimal Cu and Zn Binding Site Sequence in Amyloid Beta Peptides” *J. Biol. Chem.* **283**: 10784-10792 (2008).
40. S. Morante. “The rôle of metals in  $\beta$ -amyloid peptide aggregation: X-ray spectroscopy and numerical simulations” *Curr. Alz. Res.* **5(6)**: 508-524 (2008) **invited review**

41. S. Furlan, F. Guerrieri, G. La Penna, S. Morante, G.C. Rossi. "Studying the Cu binding sites in the PrP N-terminal region. A test case for *ab initio* simulations" *European Biophysics Journal* **36**, 841-845 (2007).
42. S. Furlan, G. La Penna, F. Guerrieri, S. Morante, G.C. Rossi. "Ab initio simulations of Cu binding sites on the N-terminal region of PrP" *Journal of Biological Inorganic Chemistry*, **12**, 571-583 (2007).
43. S. Morante, G.C. Rossi, M. Testa. "The stress tensor of a discrete system: an exercise in Statistical Mechanics" *J. Chem. Phys.* **125**, 034101 (2006).
44. F. Stellato, G. Menestrina, M. DallaSerra, C. Potrich, R. Tomazzolli, W. Meyer-Klaucke, S. Morante. "Metal binding in amyloids beta peptides shows both intra- and inter-peptide coordination modes" *Eur. Biophys. J.* **35**, 340-351 (2006).
45. G. La Penna, S. Morante, A. Perico, G.C. Rossi. "Designing generalized statistical ensembles for numerical simulations of biopolymers" *J. Chem. Phys.* **121**, 10725-10741 (2004).
46. M. Benfatto, S. Della Longa, Z. Wu, Y. Qin, G. Pan, S. Morante. "The role of Zn in the interplay among Langmuir-Blodgett Multi-Layer and Myelin Basic Protein: a quantitative analysis of XANES spectra" *Biophysical Chemistry* **110**, 191-201 (2004).
47. S. Morante, R. González-Iglesias, C. Potrich, C. Meneghini, W. Meyer-Klaucke, G. Menestrina, M. Gasset "Inter- and Intra-octarepeat Cu(II) Site Geometries in the Prion Protein. Implication in Cu(II) binding cooperativity and Cu(II)-mediated assemblies" *J. Biol. Chem.* **279**, 11753-11759 (2004).
48. G. La Penna, V. Minicozzi, S. Morante, G.C. Rossi. "Tuning force-field parameters by pressure measurements in micro-canonical simulations" *Int. J. of Mod. Phys. C* **15**, 205-221 (2004).
49. B. Berg, G. La Penna, V. Minicozzi, S. Morante, G.C. Rossi. "Multi-canonical algorithms for folding processes" *Modeling and Simulations 1967-1972* (2003).
50. F. D'Acapito, I. Emelianov, A. Relini, P. Cavatorta, A. Gliozzi, V. Minicozzi, S. Morante, P.L. Solari, R. Rolandi. "Total external reflection X-ray absorption spectroscopy reveals Zinc coordination shell in phospholipid Langmuir-Blodgett films" *Langmuir*, **18**, 5277-5282 (2002).
51. S. Nuzzo, C. Meneghini, S. Mobilio, H. Haas, P. Riccio, P. Cavatorta, S. Morante. "An X-ray Absorption Spectroscopy study of the Zinc environment in Langmuir-Blodgett phospholipid multi-layers" *Biophys. J.* **83**, 3507-3512 (2002).
52. G. La Penna, S. Letardi, V. Minicozzi, S. Morante, G.C. Rossi, G. Salina. "A simple atomistic model to simulate the gel phase of phospho-lipid bilayers" *Eur. Phys. J. E*, **5**, 259-274 (2001).
53. S. Morante. "The Zinc environment in Langmuir-Blodgett phospholipid multi-layers" *J. Synchrotron Rad.* **8**, 975-977 (2001).
54. M. Freda, G. La Penna, V. Minicozzi, S. Morante, G. Salina. "Molecular dynamics and Hybrid Monte Carlo simulations of an AOT reverse micelle"

- Progr. Colloid. Polym. Sci.* **115**, 20-24 (2000).
55. S. Morante, G.C. Rossi, G. Salina. "A Parallel Fast Fourier Transform" *Int. J. of Mod. Phys. C* **10**, 781-805 (1999).
  56. C. Meneghini, S. Morante. "The active site structure of Tetanus Neurotoxin resolved by multiple scattering analysis in X-ray absorption spectroscopy" *Biophys. J.* **75**, 1953-1963 (1998).
  57. G. La Penna, S. Letardi, V. Minicozzi, S. Morante, G.C. Rossi, G. Salina. "Parallel computing and molecular dynamics of biological membranes" *Nucl. Phys. B* **63**, 985-987 (1998).
  58. G. La Penna, V. Minicozzi, S. Morante, G.C. Rossi, G. Salina. "Molecular dynamics with the massively APE computers" *Computer Physics Communications* **106**, 53-68, (1997).
  59. T. Castrignanò A. Colosimo, S. Morante, V. Parisi, G.C. Rossi. "A study of oligonucleotide occurrence distributions in DNA coding segments" *J. Theor. Biol.* **184**, 451-469, (1997).
  60. F. Tonello, S. Morante, O. Rossetto, G. Schiavo, C. Montecucco. "Tetanus and botulism neurotoxins: a novel group of zinc-endopeptidases" *Adv. Exp. Med. Biol.* **389**, 251-260 (1996).
  61. S. Morante, L. Furenlid, G. Schiavo, F. Tonello, R. Zwillig, C. Montecucco. "X-ray absorption spectroscopy study of zinc coordination in tetanus neurotoxin, astacin alkaline protease and thermolysin" *Eur. J. Biochem.* **235**, 606-612, (1996).
  62. F. Incardona, S. Morante, V. Parisi, G.C. Rossi. "How much homologous peptides are homologous?" *J. Theor. Biol.* **175**, 437-455 (1995).
  63. R. Strange, S. Morante, S. Stefanini, S. Hasnain, E. Chiancone, A. Desideri. "Nucleation of the iron core occurs at the three-fold channels of horse spleen apoferritin: an EXAFS study on the native and chemically-modified protein" *Bioch. Bioph. Acta* **1164**, 331-334 (1993).
  64. A. Colosimo, S. Morante, V. Parisi, G.C. Rossi. "An improved method for detection of words with unusual occurrence frequency in nucleotidic sequences" *J. Theor. Biol.* **165**, 659-672 (1993).
  65. V. Balzarotti, V. Colizzi, S. Morante, V. Parisi. "An algorithm for the identification of homologous oligopeptides between amino acidic sequences: the comparison of HIV-1 gp160 and HLA class II proteins" *Comput. Appl. Biosci.* **9.1**, 93-100 (1992).
  66. G. Menestrina, G. Belmonte, V. Parisi, S. Morante. "Structural features of the pore formed by Staphylococcus aureus  $\alpha$ - toxin inferred from chemical modification and primary structure analysis" *FEMS Microbiology Immunology* **105**, 19-28 (1992).
  67. P. Cordiali, V. Balzarotti, S. Morante, V. Parisi, O. Pugliese, B. Camponeschi, V. Colizzi. "Convergent evolution in the homology between HIV gp160 and HLA Class II molecules" *Aids Research and Human Retroviruses* **8**, 1561-1565 (1992).
  68. S. Morante, V. Parisi. "Building of structural models in peptides: a semi-

- automatic software” *Comput. Appl. Biosci.* **7**, 21-26 (1991).
69. A. Colosimo, V. Balzarotti, S. Morante, V. Parisi. “Microcomputer-assisted periodic patterns recognition in the primary structure of proteins” *Biomedica Biochimica Acta* **8/9**, 951-962 (1990).
  70. A. Desideri, H.J. Hartmann, S. Morante, U. Weser. “An EXAFS study of the copper accumulated by yeast cells” *Biology of Metals* **3**, 45-47 (1990).
  71. M. Cerdonio, S. Morante, S. Vitale, A. De Young, R.W. Noble. “The use of a superconducting magnetometer to measure spin equilibria in hemoglobin” *Journal of Molecular Liquids*, **42**, 167-174 (1989).
  72. A. Desideri, M. Falconi, V. Parisi, S. Morante, G. Rotilio. “Is the activity-linked electrostatic gradient of bovine Cu,Zn superoxide dismutases conserved in homologous enzymes irrespective of the number and distribution of charges?” *Free Radical Biology and Medicine* **5**, 313-317 (1988).
  73. S. Morante, V. Parisi, A.M. Liquori. “A direct autocorrelation test to detect quasi-periodicity in the primary structure of proteins” *Chimicaoggi maggio*, 31-32 (1988).
  74. R.W. Noble, A. De Young, S. Vitale, S. Morante, M. Cerdonio. “Studies on the linkage between spin equilibria and protein structure in carp ferric hemoglobin *Eur. J. Biochem.* **168**, 563-567 (1987).
  75. A. Bianconi, A. Congiu-Castellano, M. Dell'Aricecia, A. Giovannelli, S. Morante, E. Burattini, P.J. Durham. “Local Fe site structure in the tense-to-relaxed transition in Carp deoxyhemoglobin: a XANES (x-ray absorption near edge structure) study” *Proc. Natl. Acad. Sci. USA* **83**, 7736-7740, (1986).
  76. A. Desideri, S. Morante, D. Cocco, G. Rotilio. “A room temperature magnetic susceptibility study on the cobalt derivatives of cuprozinc superoxide dismutase” *Journal of Inorganic Bioch.* **26**, 149-152 (1986).
  77. A. Bianconi, A. Congiu-Castellano, M. Dell'Aricecia, A. Giovannelli, E. Burattini, P.J. Durham, G.M. Giacometti, S. Morante. “Determination of CO and CN bond angles by X-ray absorption near edge structure in chelated protoheme in solution” *Bioch. Bioph. Acta* **831**, 114-119 (1985).
  78. A. Bianconi, A. Congiu-Castellano, M. Dell'Aricecia, A. Giovannelli, S. Morante. “Constraints of T conformation of Carp azide hemoglobin on Fe site structure” *FEBS letters* **191**, 241-244 (1985).
  79. G.O. Morpurgo, P. Porta, A. Desideri, S. Morante. “Interaction of hexacyanoferrate(III) with some copper(II) complexes” *Inorganica Chimica Acta* **107**, 111-116 (1985).
  80. M. Cerdonio, S. Morante, D. Torresani, S. Vitale, A. De Young, R.W. Noble. “Reexamination of the evidence for paramagnetism in oxy- and carbonmonoxyhemoglobins” *Proc. Natl. Acad. Sci. USA* **82**, 102-103 (1985).
  81. A. Desideri, L. Sportelli, R. Bartucci, S. Morante. “Complexes of copper(II) dipeptides with hexacyanoferrate(III). Magnetic and spectroscopic

- properties” *Inorganica Chimica Acta* **106**, 85-87 (1985).
82. R.W. Noble, A. DeYoung, E. Di Iorio, K.H. Winterhalter, M. Cerdonio, S. Morante, S. Vitale. “Quaternary structure and spin equilibria in ferric hemoglobins: a room temperature study” *Eur. J. Biochem.* **133**, 475-478 (1983).
  83. M. Cerdonio, S. Morante, S. Vitale, C. Dalvit, M. Russu, C. Ho, A. De Young, R.W. Noble. “Magnetic and spectral properties of Carp carbonmonoxyhemoglobin” *Eur. J. Biochem.* **132**, 461-467 (1983).
  84. P. Durham, A. Bianconi, A. Congiu-Castellano, A. Giovannelli, S.S. Hasnain, L. Incoccia, S. Morante, J.P. Pendry. “X-ray absorption near edge structure (XANES) for CO, CN and deoxyhaemoglobin: geometrical information” *EMBO J.* **9**, 1441-1443 (1983).
  85. S. Vitale, S. Morante, M. Cerdonio. “Superconducting susceptometer for high-accuracy routine operation” *Rev. Sci. Instrum.* **53**, 1123-1128 (1982).
  86. M. Cerdonio, S. Morante, S. Vitale. “Low Lying paramagnetic states in oxy- and carbonmonoxyhemoglobins” *Israel Journal of Chemistry* **21**, 76-80 (1981).
  87. M. Cerdonio, S. Morante, S. Vitale, E.E. Di Iorio, K.H. Winterhalter, G.M. Giacometti, M. Brunori. “Magnetic equivalence of the hemes in hemoglobin Zurich” *J. Biol. Chem.* **255**, 6166-6167 (1980).
  88. M. Cerdonio, S. Morante, S. Vitale, A. De Young, R.W. Noble. “Variability of the magnetic moment of carbon monoxide hemoglobin from carp” *Proc. Natl. Acad. Sci. USA* **77**, 1462-1465 (1980).
  89. M. Cerdonio, S. Morante, M. Vicentini-Missoni. “Polar growth response of *Pisum Arvense* L. seeds to weak magnetic fields” *Can. J. Plant. Sci.* **59** 883-885 (1979).
  90. M. Cerdonio, A. Congiu-Castellano, L. Calabrese, S. Morante, B. Pispisa, S. Vitale. “Room temperature magnetic properties of oxy- and carbonmonoxyhemoglobin” *Proc. Natl. Acad. Sci. USA* **75**, 4916-4919 (1978).

### Peer Reviewed Proceedings

91. V. Minicozzi, S. Morante, G.C. Rossi, F. Stellato. “The rôle of Metals in Amyloid Aggregation: A Test Case for ab initio Simulations” *Comp. Mod. Sci. and Eng.* **963**: 92-97 (2007).
92. V. Minicozzi, S. Morante, G.C. Rossi, F. Stellato, K. Jansen, “The role of metals in misfolding and aggregation processes: X-ray spectroscopy and numerical simulations” in “*From Computational Biophysics to System Biology*”, ed. by J. Meinke, O. Zimmermann, S. Mohanty, U.H.E. Hansmann, *NIC Series*, **36**, 223-225 (2007).
93. S. Furlan, F. Guerrieri, G. La Penna, S. Morante, G.C. Rossi, “Ab initio simulations of Cu binding sites in the N-terminal region of PrPs” in “*From*

- Computational Biophysics to System Biology*”, ed. by J. Meinke, O. Zimmermann, S. Mohanty, U.H.E. Hansmann, *NIC Series*, **34**, 153-156 (2006).
94. G. Menestrina, M. Comai, C. Potrich, M. DallaSerra, G. Guella, R. Frassanito, C. Meneghini, S. Mobilio, S. Morante. “Metal ions and the conformation of peptides forming amyloid deposits in Alzheimer and prion disease”. *Acta Cryst. A* **58**, C245 (2002).
  95. S. Morante et al. “Design study of a soft X-ray SASE-FEL source” *8th European Particle Accelerator Conference*, 825-827 (2002).
  96. G. La Penna, V. Minicozzi, S. Morante, G.C. Rossi, G. Salina. “Molecular dynamics with APE” in *"Multiscale Phenomena and their Simulation"* World Scientific Publishing, London UK, 129-135 (1997).
  97. A. Congiu-Castellano, A. Bianconi, M. Dell'Ariceia, A. Giovannelli, S. Della Longa, E. Burattini, G. Giacometti, S. Morante. “Ligand binding angle in hemoproteins by XANES spectroscopy” in *"Synchrotron Radiation at Frascati: 1986 users meeting"* ed. by S. Mobilio, F. Patella, S. Stipcich. Italian Physical Society, Bologna, 67-69 (1986).
  98. A. Desideri, S. Morante, D. Cocco, G. Rotilio. “An EXAFS study of chloride binding to oxidized and reduced superoxide dismutase” in *"Synchrotron Radiation at Frascati: 1986 users meeting"* ed. by S. Mobilio, F. Patella, S. Stipcich. Italian Physical Society, Bologna, 85-86 (1986).
  99. M. Cerdonio, S. Morante, S. Vitale. “High accuracy superconducting magnetometer” in *Int. Cryo. Eng. Conf.*, ed. by C. Rizzuto, IPC Science and Technology Press, Guildford, UK, 443-446 (1980).
  100. M. Cerdonio, S. Morante, S. Vitale. “A superconducting susceptometer measuring total magnetic moments” *Int. Conf. Ref.* **A1/2-30.1-A1/2-30.5** (1979).

### Invited reviews and book's chapters

101. BioFEL Collaboration - spokesperson Silvia Morante “FEL's light into life: The value of SPARX for life sciences” (2009) <http://www.sparx-fel.it/index.php/en/sparx-science/scientific-case>
102. S. Morante. “Metal ions and protein aggregation: the case of Prion protein and  $\beta$ -amyloids” **invited review** in *"Biophysical Inquiry into Protein Aggregation and Amyloid Diseases"*, eds. D. Bulone and P.L. San Biagio, *Research Signpost Edition*, Ch. **3** (2008).
103. S. Morante, C. Meneghini. “Resolving the structure of Tetanus Neurotoxin by X-ray Absorption Spectroscopy” *INFM Highlights 1998/1999*, 22-24 (2001).
104. H. Haas, S. Nuzzo, S. Pascarelli, P. Cavatorta, S. Morante, P. Riccio, S. Mobilio. “X-ray absorption spectroscopy study of zinc coordination in Langmuir-Blodgett layers from phospholipids and myelin basic protein.”

*ESRF Highlights 1997-98*, 29-30 (1999).

105. A.Desideri, S. Morante, G. Rotilio. "The active site of Cu,Zn superoxide dismutase studied by EXAFS: the binding of chloride to the reduced enzyme" in "*Biophysics and Synchrotron radiation*" ed. by A. Bianconi, A. Congiu-Castellano, Springer Verlag, Berlin, **2**, 159-163 (1987).
106. S. Morante, A. Congiu-Castellano, M. Dell'Aricecia, P.J. Durham, A. Giovannelli, E. Burattini, A. Bianconi. "The high and low spin iron sites and the T to R transition in carp hemoglobin" in "*Biophysics and Synchrotron radiation*" ed. by A. Bianconi, A. Congiu-Castellano, Springer Verlag, Berlin, **2**, 107-113 (1987).
107. A.Desideri, S. Morante, D. Cocco, G. Rotilio. "An EXAFS study at the copper K edge of the derivative of bovine Superoxide Dismutase modified in the zinc site", in "*Superoxide and Superoxide Dismutase in chemistry biology and medicine*" ed by G. Rotilio, 161-164 (1986)
108. M. Cerdonio, S. Morante, S. Vitale, G. Giacometti, M. Brunori. "Spin unpairing in oxy- and carbonmonoxy-hemoglobins" in "*Interaction between iron and proteins in oxygen and electron transport*", ed. by Chien Ho, Elsevier North Holland, Amsterdam, The Netherland, 63-67 (1982).
109. S. Morante, M. Cerdonio, S. Vitale, A. Congiu-Castellano, A. Vaciago, G.M. Giacometti, L. Incoccia. "X-ray iron K edge of human hemoglobins" in "*EXAFS and near edge structure*", ed. by A. Bianconi, L. Incoccia, S. Stipcich, Springer Verlag, Berlin, Germany, 352-354 (1982).
110. M. Cerdonio, S. Morante, S. Vitale. "Magnetic susceptibility of hemoglobins", in "*Hemoglobin*" a volume of "*Methods in Enzimology*", ed. by S.P. Colowick, N.O. Kaplan. Academic Press (copyright Elsevier Science Publisher in Amsterdam - The Netherlands) **76**, 354-371 (1981).
111. M. Cerdonio, S. Morante, S. Vitale. "Magnetic properties and structure of oxyhemoglobin and carbonmonoxyhemoglobin" in "*Biophysical Research*" ed. by A. Borsellino, P. Omodeo, R. Strom, A. Vecli, E. Wanke. Plenum Press, New York and London, 249-257 (1979).