

## List of publications

**Silvia Morante**

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

1. 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.2018.04.134
2. 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>
3. 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
4. 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**
5. 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
6. 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
7. 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
8. 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

9. 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
10. E. De Santis, V. Minicozzi, O. Proux, G. C. Rossi, K. I. Silva, M.J. Lawless, F. Stellato, S. Saxena and S. Morante "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
  - a. doi: 10.1021/acs.jpcc.5b10264
11. 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
12. 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)
13. 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.
14. 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.
15. 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
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17. 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.* (2013) **A740**, 138-146 DOI: [10.1016/j.nima.2013.11.040](https://doi.org/10.1016/j.nima.2013.11.040)
18. 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
19. 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
20. 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:
21. 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
22. F. Stellato, A. Spevacek, O. Proux, V. Minicozzi, G. Millhauser, S. Morante “Zinc modulates Copper coordination mode in Prion Protein octarepeat subdomains” *European Biophysical Journal* **40**: 1259-1270 (2011). DOI: 10.1007/s00249-011-0713-4
23. 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) .
24. V. Minicozzi, S. Morante. “Is Cu involved in prion oligopeptide stability? Experiments and numerical simulations.” *International Journal of Quantum Chemistry* **110**: 656-680 (2010).
25. 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).
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27. 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). doi:10.1007/s00775-008-0454-8
28. 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). DOI: 10.1002/qua.21724
29. 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). ISBN: 8178953544,

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30. 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). DOI: [10.1074/jbc.M707109200](https://doi.org/10.1074/jbc.M707109200)
31. 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 DOI: <https://doi.org/10.2174/156720508786898505>
32. 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). Doi: 10.1007/s00249-007-0162-2
33. 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). doi: <http://dx.doi.org/10.1063/1.2836245>
34. 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). ISBN 978-3-9810843-2-0,
35. 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). Doi: 10.1007/s00775-007-0218-x
36. 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). doi: <http://dx.doi.org/10.1063/1.2214719>
37. 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). 10.1007/s00249-005-0041-7
38. 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).
39. 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). doi: <http://dx.doi.org/10.1063/1.1795694>
40. 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). <https://doi.org/10.1016/j.bpc.2004.02.003>
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  43. G.I. Giannoli, S.Morante, R. Mordenti, P.Quintili. “Culture per la Pace” Manifesto Libri Srl ISBN: 8872853559
  44. 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). DOI: 10.1021/la025564q
  45. 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). doi: [10.1016/S0006-3495\(02\)75350-2](https://doi.org/10.1016/S0006-3495(02)75350-2)
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## **85. Peer Reviewed Proceedings**

86. B. Berg, G. La Penna, V. Minicozzi, S. Morante, G.C. Rossi. "Multi-canonical algorithms for folding processes" *Modeling and Simulations* 1967-1972 (2003).
87. G. Menestrina, M. Comai, C. Potrich, M. DallaSerra, G. Guella, R. Frasanito, C. Meneghini, S. Mobilio, S. Morante. "Metal ions and the conformation of peptides forming amyloid deposits in Alzheimer and prion disease". *Acta Cryst.* **A58**, C245 (2002).
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#### 94. Invited reviews and book's chapters

95. 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>
96. S. Morante, C. Meneghini. "Resolving the structure of Tetanus Neurotoxin by X-ray Absorption Spectroscopy" *INFM Highlights 1998/1999*, 22-24 (2001).
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