I. CURRICULUM VITAE OF GIORDANO MANCINI

NAME	PERSONAL INFORMATION
Giordano, MANCINI	• I [illegible] June 1979 in [illegible] • e-mail: giordano.mancini@sns.it •

PRESENT POSITION

- Chief Operating Office, SMART Laboratory, Scuola Normale Superiore

EDUCATION/PAST POSITIONS

INSTITUTION AND LOCATION	DEGREE *(if applicable)*	YEAR(s)
Scuola Normale Superiore, Pisa, Italy, (Post Doc fellow)		2013-2017
Scuola Normale Superiore, Pisa, Italy, (Post Doc fellow)		2012-2013
Università degli studi della Tuscia, Viterbo, Italy		2009-2012
CNR/IMIP Bari, Italy (Post Doc fellow)		2007-2008
Università La Sapienza di Roma (Rome, Italy)/CASPUR	Ph. D. Physical Chemistry	2004-2007
Università La Sapienza di Roma (Rome, Italy)	B. Sc./M. Sc Chemistry (cum laude)	1998-2004

A. Synopsis of research activity (updated September 2017)

Ph. D. Thesis in Physical Chemistry:
"A combined computational and XAS approach to the study of structural and dynamical properties of electrolitic aqueous solutions"

Publication activity

60 papers on peer-reviewed journals (15 as first and/or corresponding author), 2 book chapters; 910 citations; H-index: 19

Research grants

- Awarded an institutional Research Grant from host institution "In silico design of new fluorescent molecular rotors"
- Awarded a national research grant (unit coordinator) for the project "Nanotubi di argilla per la progettazione di materiali intelligenti ecosostenibili". Bando "FIRB Futuro in Ricerca bando 2012".
- Awarded an institutional Research Grant from host institution "Supporto alla ricerca di base"

Current Research Interests

- Application of XAS spectroscopy and Classical Molecular Dynamics to the study of metallo-proteins with focus on the structural effects due to the binding of molecules such as CO or NO or metal ions (e.g. Cu^{2+}).
- Development of algorithms for MD simulations in Non-periodic Boundary Conditions. Application of Polarizable force fields. Development of accurate parametrization of classical force fields
- Graphical interfaces and immersive/interactive tools for Molecular Modeling.

Institutional web sites: http://smart.sns.it/?pag=vmd, http://smart.sns.it/?pag=hpc

B. Teaching

Teaching activity

- Course "Introduction to Scientific Calculus, Scuola Normale Superiore", 2016-2017
- Course "Programming Languages for Chemists", Scuola Normale Superiore 2013-2015
- Course "Computational modeling of Bio- and nano-sistems", Scuola Normale Superiore 2013-2014
- Course in "Molecular Dynamics of Biological macromolecules", CASPUR 2011-2012
- Lectures in "Computational Biology", Tor Vergata University (2010)

C. Programming skills and software

- Sys-admin level knowledge of GNU/Linux OS. Management of Beowulf clusters. Use of Bright Cluster Manager
- Programming Languages: Python [Pandas, Sci-kit Learn], C/C++, Fortran

77/90, AWK (very good); R, Perl (good)

- Database management system: MySQL
- Parallel programming with MPI/OpenMP. Basic knowledge of CUDA and OpenAcc
- Molecular modeling software: Gaussian09, GROMACS, NWChem, AMBER, NAMD, Chimera, VMD
- Publishing software: GIMP, Blender, Inkscape

D. Additional formation, winter/summer schools

- Ottimizzazione di codici numerici seriali e paralleli: Corso CASPUR Novembre 2005
- Debugging di codici seriali Corso: CASPUR Ottobre 2005
- "A two day course on MPI" Edimburgh Parallel Computing Centre (EPCC), Edimburgh, UK, May 2007
- "Understanding Molecular Simulations", Universeit Van Amsterdam (UVA), Amsterdam, NL, 08-19 Jan 2007
- Statistical methods for genome-enabled selection: Summer School, Università di Padova. Sept 2010
- INFN Efficiency in Scientific Computing School, Nov 2013
- Introduction to Machine Machine Learning (Coursera) 2016
- Statistical Learning (2016)
- Clustering in Data Mining (Coursera) 2016
- 9 Measure shifts at various synchrotron radiation facilities in Europe between 2005 and 2015

E. Publication activity

E.1 Papers Submitted and under review

1. A. Salvadori, M. Fusé, G. Mancini, S. Rampino, V. Barone Diving into chemical bonding: an immersive analysis of the electron charge rearrangement through virtual reality. Submitted to *Journal of Computational Chemistry*
2. D. Licari, M. Fusé, A. Salvadori, M. Mendolicchio, N. Tasinato, G. Mancini, V. Barone Towards the SMART workflow for Computational Spectroscopy. Invited perspective to *Physical Chemistry Chemical Physics*

E.2 Published papers

1. B. Chandramouli; S. Del Galdo; G. Mancini; N. Tasinato; V. Barone. Tailor-Made Computational Protocols for Precise Characterization of Small Biological Building Blocks Using QM and MM Approaches. Biopolymers 2018, e23109.
2. S. Del Galdo; G. Mancini; I. Daidone; L. Zanetti Polzi; A. Amadei; V. Barone Tyrosine Absorption Spectroscopy: Backbone Protonation Effects on the Side Chain Electronic Properties. Journal of Computational Chemistry 2018.
3. F. Sessa, V. Migliorati, A. Serva, A. Lapi, G. Aquilanti, G. Mancini and P. D'Angelo, On the coordination of Zn 2+ ion in Tf 2 N − based ionic liquids: structural and dynamic properties depending on the nature of the organic cation, Physical Chemistry Chemical Physics, , DOI:10.1039/C7CP07497B.
4. F. Fracchia, G. Del Frate, G. Mancini, W. Rocchia and V. Barone, Force Field Parametrization of Metal Ions from Statistical Learning Techniques, Journal of Chemical Theory and Computation, 2018, 14, 255–273.
5. J. L. Williams, D. Iamartino, K. D. Pruitt, T. Sonstegard, T. P. L. Smith, W. Y. Low, T. Biagini, L. Bomba, S. Capomaccio, B. Castiglioni, A. Coletta, F. Corrado, F. Ferré, L. Iannuzzi, C. Lawley, N. Macciotta, M. McClure, G. Mancini, D. Matassino, R. Mazza, M. Milanesi, B. Moioli, N. Morandi, L. Ramunno, V. Peretti, F. Pilla, P. Ramelli, S. Schroeder, F. Strozzi, F. Thibaud-Nissen, L. Zicarelli, P. Ajmone-Marsan, A. Valentini, G. Chillemi and A. Zimin, Genome assembly and transcriptome resource for river buffalo, Bubalus bubalis (2n = 50), GigaScience, , DOI:10.1093/gigascience/gix088.
6. M. Macchiagodena, G. Mancini, M. Pagliai, G. Cardini and V. Barone, New atomistic model of pyrrole with improved liquid state properties and structure., International Journal of Quantum Chemistry, 2017, e25554.
7. M. Macchiagodena, G. Mancini, M. Pagliai, G. Del Frate and V. Barone, Fine-tuning of atomic point charges: classical simulations of pyridine in different environments, Chemical Physics Letters, , DOI:10.1016/j.cplett.2017.04.004.
8. M. Macchiagodena, G. Del Frate, G. Brancato, B. Chandramouli, G. Mancini and V. Barone, Computational study of the DPAP molecular rotor in various environments: from force field development to molecular dynamics simulations and spectroscopic calculations, Physical Chemistry Chemical Physics, 2017, 19, 30590–30602.
9. O. Carrillo-Parramon, S. del Galdo, M. Aschi, G. Mancini, A. Amadei and V. Barone, Flexible and Comprehensive Implementation of MD-PMM Approach in a General and Robust Code, Journal of Chemical Theory and Computation, , DOI:10.1021/acs.jctc.7b00341.
10. A. Salvadori, G. Del Frate, M. Pagliai, G. Mancini and V. Barone, Immersive virtual reality in computational chemistry: Applications to the analysis of QM and MM data, International Journal of Quantum Chemistry, , DOI:10.1002/qua.25207.
11. D. Presti, A. Pedone, G. Mancini, C. Duce, M. R. Tiné and V. Barone, Insights into structural and dynamical features of water at halloysite interfaces probed by DFT and classical molecular dynamics simulations, Phys. Chem. Chem. Phys., 2016, 18, 2164–2174.
12. M. Pagliai, G. Mancini, I. Carnimeo, N. De Mitri and V. Barone, Electronic absorption spectra of pyridine and nicotine in aqueous solution with a combined molecular dynamics and polarizable QM/MM approach, Journal of Computational Chemistry, , DOI:10.1002/jcc.24683.
13. M. Olszówka, R. Russo, G. Mancini and C. Cappelli, A computational approach to the resonance Raman spectrum of doxorubicin in aqueous solution, Theoretical Chemistry Accounts, , DOI:10.1007/s00214-015-1781-9.
14. M. Macchiagodena, G. Mancini, M. Pagliai and V. Barone, Accurate prediction of bulk

properties in hydrogen bonded liquids: amides as case studies, Phys. Chem. Chem. Phys., , DOI:10.1039/C6CP04666E.
15. G. Del Frate, F. Bellina, G. Mancini, G. Marianetti, P. Minei, A. Pucci and V. Barone, Tuning of dye optical properties by environmental effects: a QM/MM and experimental study, Phys. Chem. Chem. Phys., 2016, 18, 9724–9733.
16. P. D'Angelo, V. Migliorati, F. Sessa, G. Mancini and I. Persson, XANES Reveals the Flexible Nature of Hydrated Strontium in Aqueous Solution, The Journal of Physical Chemistry B, 2016, 120, 4114–4124.
17. G. Mancini and C. Zazza, F429 Regulation of Tunnels in Cytochrome P450 2B4: A Top Down Study of Multiple Molecular Dynamics Simulations, PLOS ONE, 2015, 10, e0137075.
18. G. Mancini, G. Brancato, B. Chandramouli and V. Barone, Organic solvent simulations under non-periodic boundary conditions: A library of effective potentials for the GLOB model, Chemical Physics Letters, , DOI:10.1016/j.cplett.2015.03.001.
19. G. Giachin, P. T. Mai, T. H. Tran, G. Salzano, F. Benetti, V. Migliorati, A. Arcovito, S. D. Longa, G. Mancini, P. D'Angelo and G. Legname, The non-octarepeat copper binding site of the prion protein is a key regulator of prion conversion, Scientific Reports, 2015, 5, 15253.
20. F. Egidi, R. Russo, I. Carnimeo, A. D'Urso, G. Mancini and C. Cappelli, The Electronic Circular Dichroism of Nicotine in Aqueous Solution: a Test Case for Continuum and Explicit-Continuum Solvation Approaches, The Journal of Physical Chemistry A, 2015, 150108134059007.
21. B. Chandramouli, C. Zazza, G. Mancini and G. Brancato, Boundary Condition Effects on the Dynamic and Electric Properties of Hydration Layers, The Journal of Physical Chemistry A, 2015, 150318104422003.
22. B. Chandramouli, D. Di Maio, G. Mancini and G. Brancato, Introducing an artificial photo-switch into a biological pore: A model study of an engineered α-Hemolysin, Biochimica et Biophysica Acta (BBA) - Biomembranes, , DOI:10.1016/j.bbamem.2015.12.030.
23. B. Chandramouli, D. Di Maio, G. Mancini, V. Barone and G. Brancato, Breaking the Hydrophobicity of the MscL Pore: Insights into a Charge-Induced Gating Mechanism, PLOS ONE, 2015, 10, e0120196.
24. A. Salvadori, A. Brogni, G. Mancini and V. Barone, in Augmented and Virtual Reality, eds. L. T. De Paolis and A. Mongelli, Springer International Publishing, Cham, 2014, vol. 8853, pp. 333–350.
25. G. Mancini, G. Brancato and V. Barone, Combining the Fluctuating Charge Method, Non-periodic Boundary Conditions and Meta-dynamics: Aqua Ions as Case Studies, Journal of Chemical Theory and Computation, 2014, 140221073102006.
26. P. D'Angelo, V. Migliorati, I. Persson, G. Mancini and S. D. Longa, Quantitative Analysis of Deconvolved X-ray Absorption Near-Edge Structure Spectra: A Tool To Push the Limits of the X-ray Absorption Spectroscopy Technique, Inorganic Chemistry, 2014, 140829151720009.
27. C. Zazza, G. Mancini, G. Brancato and V. Barone, In Silico Study of Molecular-Engineered Nanodevices: A Lockable Light-Driven Motor in Dichloromethane Solution, The Journal of Physical Chemistry Letters, 2013, 3885–3890.
28. V. Migliorati, G. Mancini, S. Tatoli, A. Zitolo, A. Filipponi, S. De Panfilis, A. Di Cicco and P. D'Angelo, Hydration Properties of the Zn 2+ Ion in Water at High Pressure, Inorganic Chemistry, 2013, 52, 1141–1150.
29. C. Zazza, G. Mancini, G. Brancato, N. Sanna and V. Barone, Neutral molecular shuttle in acetonitrile dilute solution investigated by molecular dynamics and density functional theory,

Computational and Theoretical Chemistry, 2012, 985, 53–61.
30. G. Mancini, I. D'Annessa, A. Coletta, G. Chillemi, Y. Pommier, M. Cushman and A. Desideri, Binding of an Indenoisoquinoline to the Topoisomerase-DNA Complex Induces Reduction of Linker Mobility and Strengthening of Protein-DNA Interaction, PLoS ONE, 2012, 7, e51354.
31. P. D'Angelo, S. Della Longa, A. Arcovito, G. Mancini, A. Zitolo, G. Chillemi, G. Giachin, G. Legname and F. Benetti, Effects of the Pathological Q212P Mutation on Human Prion Protein Non-Octarepeat Copper-Binding Site, Biochemistry, 2012, 51, 6068–6079.
32. G. Chillemi, S. De Santis, M. Falconi, G. Mancini, V. Migliorati, A. Battistoni, F. Pacello, A. Desideri and P. D'Angelo, Carbon monoxide binding to the heme group at the dimeric interface modulates structure and copper accessibility in the Cu,Zn superoxide dismutase from Haemophilus ducreyi : in silico and in vitro evidences, Journal of Biomolecular Structure and Dynamics, 2012, 30, 269–279.
33. V. Migliorati, G. Mancini, G. Chillemi, A. Zitolo and P. D'Angelo, Effect of the Zn 2+ and Hg 2+ Ions on the Structure of Liquid Water, The Journal of Physical Chemistry A, 2011, 115, 4798–4803.
34. G. Mancini, C. Zazza, M. Aschi and N. Sanna, Conformational analysis and UV/Vis spectroscopic properties of a rotaxane-based molecular machine in acetonitrile dilute solution: when simulations meet experiments, Physical Chemistry Chemical Physics, 2011, 13, 2342.
35. P. D'Angelo, A. Zitolo, V. Migliorati, E. Bodo, G. Aquilanti, J. L. Hazemann, D. Testemale, G. Mancini and R. Caminiti, X-Ray absorption spectroscopy investigation of 1-alkyl-3-methylimidazolium bromide salts, The Journal of Chemical Physics, 2011, 135, 074505.
36. C. Zazza, G. Mancini, A. Amadei, N. Sanna and M. Aschi, A fast redox-induced switching mechanism in a conformationally controllable molecular thread in solution, Physical Chemistry Chemical Physics, 2010, 12, 4552.
37. C. Zazza, A. Coletta, N. Sanna, G. Chillemi, G. Mancini and A. Desideri, Solvent Effects on the Valence UV−Vis Absorption Spectra of Topotecan Anticancer Drug in Aqueous Solution at Room Temperature: A Nanoseconds Time-Scale TD-DFT/MD Computational Study, The Journal of Physical Chemistry B, 2010, 114, 6770–6778.
38. G. Mancini, I. D'Annessa, A. Coletta, N. Sanna, G. Chillemi and A. Desideri, Structural and Dynamical Effects Induced by the Anticancer Drug Topotecan on the Human Topoisomerase I – DNA Complex, PLoS ONE, 2010, 5, e10934.
39. P. D'Angelo, A. Zitolo, F. Pacello, G. Mancini, O. Proux, J. L. Hazemann, A. Desideri and A. Battistoni, Fe-heme structure in Cu,Zn superoxide dismutase from Haemophilus ducreyi by X-ray Absorption Spectroscopy, Archives of Biochemistry and Biophysics, 2010, 498, 43–49.
40. C. Zazza, G. Mancini, N. Sanna and M. Aschi, Thermodynamic features and environmental effects in a two-states molecular device under strict electrochemical control, Theoretical Chemistry Accounts, 2009, 123, 383–390.
41. N. Sanna, G. Chillemi, L. Gontrani, A. Grandi, G. Mancini, S. Castelli, G. Zagotto, C. Zazza, V. Barone and A. Desideri, UV−Vis Spectra of the Anticancer Campothecin Family Drugs in Aqueous Solution: Specific Spectroscopic Signatures Unraveled by a Combined Computational and Experimental Study, The Journal of Physical Chemistry B, 2009, 113, 5369–5375.
42. M. Rutigliano, C. Zazza, N. Sanna, A. Pieretti, G. Mancini, V. Barone and M. Cacciatore, Oxygen Adsorption on β-Cristobalite Polymorph: Ab Initio Modeling and Semiclassical Time-Dependent Dynamics †, The Journal of Physical Chemistry A, 2009, 113, 15366–

15375.
43. F. Ramondo, L. Tanzi, M. Campetella, L. Gontrani, G. Mancini, A. Pieretti and C. Sadun, Hydration of diazoles in water solution: pyrazole. A theoretical and X-ray diffraction study, Physical Chemistry Chemical Physics, 2009, 11, 9431.
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47. P. D'Angelo, A. Zitolo, V. Migliorati, G. Mancini, I. Persson and G. Chillemi, Structural Investigation of Lanthanoid Coordination: a Combined XANES and Molecular Dynamics Study, Inorganic Chemistry, 2009, 48, 10239–10248.
48. G. Chillemi, A. Coletta, G. Mancini, N. Sanna and A. Desideri, An amber compatible molecular mechanics force field for the anticancer drug topotecan, Theoretical Chemistry Accounts, 2009, 127, 293–302.
49. G. Mancini, N. Sanna, V. Barone, V. Migliorati, P. D'Angelo and G. Chillemi, Structural and Dynamical Properties of the Hg 2+ Aqua Ion: A Molecular Dynamics Study, The Journal of Physical Chemistry B, 2008, 112, 4694–4702.
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51. P. D'Angelo, V. Migliorati, G. Mancini and G. Chillemi, A Coupled Molecular Dynamics and XANES Data Analysis Investigation of Aqueous Cadmium(II), The Journal of Physical Chemistry A, 2008, 112, 11833–11841.
52. A. Arcovito, T. Moschetti, P. D'Angelo, G. Mancini, B. Vallone, M. Brunori and S. Della Longa, An X-ray diffraction and X-ray absorption spectroscopy joint study of neuroglobin, Archives of biochemistry and biophysics, 2008, 475, 7–13.
53. G. Chillemi, G. Mancini, N. Sanna, V. Barone, S. D. Longa, M. Benfatto, N. V. Pavel and P. D'Angelo, Evidence for Sevenfold Coordination in the First Solvation Shell of Hg(II) Aqua Ion, Journal of the American Chemical Society, 2007, 129, 5430–5436.
54. P. D'Angelo, F. Pacello, G. Mancini, O. Proux, J. L. Hazemann, A. Desideri and A. Battistoni, X-ray Absorption Investigation of a Unique Protein Domain Able To Bind both Copper(I) and Copper(II) at Adjacent Sites of the N-Terminus of Haemophilus ducreyi Cu,Zn Superoxide Dismutase †, Biochemistry, 2005, 44, 13144–13150.
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56. G. Chillemi, V. Barone, P. D'Angelo, G. Mancini, I. Persson and N. Sanna, Computational Evidence for a Variable First Shell Coordination of the Cadmium(II) Ion in Aqueous Solution, The Journal of Physical Chemistry B, 2005, 109, 9186–9193.