# Isabella Daidone Curriculum Vitae


Address: University of L'Aquila
Via Vetoio (Coppito 1)
67010 Coppito (AQ) - Italy

Nationality: Italian, Finnish
Email: isabella.daidone@univaq.it


## Current position

Current position **Permanent Research Scientist** at the department of Physical and Chemical Sciences of the University of L'Aquila (Italy).

## Research Interests

- Simulations of molecular and macromolecular systems with classical and combined quantum/classical methods
- Thermodynamics and statistical mechanics of molecular systems in general and more specifically of protein folding
- Kinetic models of protein folding and diffusion
- Algorithms for enhanced molecular dynamics sampling of proteins (Essential Dynamics Sampling)
- Theoretical studies of chemical reactions in proteins
- Neutron scattering, infrared and fluorescence spectroscopies applied to biomolecules

## Scientific Education

October 2004 **Ph.D. in Chemistry**
University of Rome "La Sapienza" (Italy)
Research project: *Study of folding and misfolding processes by the use of computational methods*
Supervisor: Prof. Alfredo Di Nola

May 2001 **Degree (Laurea) in Chemistry - Summa cum laude**
University of Rome "La Sapienza" (Italy)
Thesis: *Simulazioni di dinamica molecolare del citocromo c*
Supervisor: Prof. Alfredo Di Nola

July 1993 **High School Diploma (Maturità Scientifica) – 60/60**
Liceo "G.B. Morgagni", Rome (Italy)

## Further Scientific Experience

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| June 2007 – Feb. 2009 | **Marie Curie fellow (individual fellowship)** at the "*Computational Molecular Biophysics Group*" of Prof. Jeremy C. Smith, IWR, Uni Heidelberg (Germany). |
| June 2005 – May 2007 | **Post Doctoral position** at the "*Computational Molecular Biophysics Group*" of Prof. Jeremy C. Smith, IWR, University of Heidelberg (Germany). |
| Nov. 2004 – May 2005 | **Post Doctoral position** at the "*Theoretical and Computational Physical Chemistry Group*" of Prof. Alfredo Di Nola, University of Rome "La Sapienza" (Italy). |
| June 2007 | Visitor researcher at the "*Spallation Neutron Source*" and the "*Center for Molecular Biophysics*", Oak Ridge National Laboratory - ORNL, Tennesse (USA). |
| Since July 2006 | Collaboration with the "*Applied Laserphysics & Laserspectroscopy*" group of Prof. Markus Sauer, department of physics, University of Bielefeld (Germany). |
| Jan. 2001 – May 2005 | Collaboration with Dr. Giorgio Colombo, *"Istituto di Chimica del Riconoscimento Molecolare"* - CNR, Milano (Italy), and with Prof. Ehud Gazit, department of *"Molecular Microbiology and Biotechnology",* University of Tel Aviv (Israel). |
| July 2003 | Visitor researcher at the "*School of Computing Sciences*", group of Dr. Steven Hayward, University of East Anglia, Norwich (UK). |
| July 2002 | Attendance to the *"11ª Summer school on parallel computing"*, CINECA, Casalecchio di Reno - BO (Italy). |
| Jan. 2001 – April 2001 | Attendance to the course: "*A hierarchy of models for simulating the real world*" held by Prof. H.J.C. Berendsen of the University of Gröningen (NL). |

## Teaching

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| 2008-2013 | Lecturer: , "*Metodi Computazionali*", Department of Chemistry, University of L'Aquila, Italy. |
| 2008-2012 | Lecturer: "*Chimica Inorganica Superiore*", Department of Chemistry, University of L'Aquila, Italy. |
| 12 Oct. 2007 | Lecturer: "*Protein folding in silico*" (within the program "*BioNoCo – Biocatalysis using non-conventional media*"), Forschungszentrum Jülich GmbH**,** Jülich (Germany). |
| Summer 2007 | Lecturer: "*Structural Biology Weekend Seminar*", IWR, University of Heidelberg (Germany). |
| 2006-2008 | Lecturer: "*Introduction to (bio)-molecular modeling and simulation*", University of Heidelberg (Germany). |

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| 2001 - 2004 | Teaching Assistant: Chemistry Department, University of Rome "La Sapienza" (Italy). Courses: "*Computational Chemistry*", "*Elements of Chemical Informatics*", "*Mathematics*". |
| 2002 - 2004 | Teaching Assistant: MASTER in "*Bioinformatica: applicazioni biomediche e farmaceutiche*", Biochemistry Department “A. Ross Fanelli”, University of Rome "La Sapienza" (Italy) |

## Supervision of students

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| Sep. 2011– July 2012 | Diploma thesis: Giuseppe Guarracino<br>Department of Chemistry, University of L'Aquila, Italy.<br>Status: Completed |
| Mar. 2011– Mar. 2012 | Diploma thesis: Andrea Le Donne<br>Department of Chemistry, University of L'Aquila, Italy.<br>Status: Completed |
| Oct. 2009 – Oct. 2010 | Diploma thesis: Claudio Iacobucci<br>Department of Chemistry, University of L'Aquila, Italy.<br>Status: Completed |
| Jan. 2007 – July 2011 | PhD thesis: Lipi Thukral<br>"*Computational Molecular Biophysics Group*", IWR, Uni Heidelberg, Germany.<br>Status: Completed |
| May 2006 – April 2007 | Diploma thesis: Roland Schulz (with Prof. Jeremy C. Smith)<br>"*Computational Molecular Biophysics Group*", IWR, Uni Heidelberg, Germany.<br>Status: Completed |
| March 2004 – July 2005 | Diploma thesis: Giulia Rossetti (with Prof. Alfredo Di Nola)<br>Department of Chemistry, University of Rome "La Sapienza", Italy.<br>Status: Completed |
| Gen. 2004 – May 2005 | Diploma thesis: Daniele Narzi (with Prof. Alfredo Di Nola)<br>Department of Chemistry, University of Rome "La Sapienza", Italy.<br>Status: Completed |

## Selected publications


**1** Bortolotti C.A., Amadei A., Aschi M., Borsari M., Corni S., Sola M. and Daidone I.* *The reversible opening of two water channels in cytochrome c modulates the redox potential.* **J. Am. Chem. Soc**. 2012, 134:13670-13678.

**2** Zanetti-Polzi L., Amadei A., Aschi M. and Daidone I.* *Insight into the IR-spectra/structure relationship in amyloid fibrils: a theoretical study on a prion peptide.* **J. Am. Chem. Soc.** 2011, 133:11414-11417.

**3** Daidone I.*, Di Nola A.* and Smith J.C. *Molecular origin of Gerstmann-Strässler-Scheinker syndrome: insight from computer simulation of an amyloidogenic prion peptide.* **Biophys. J.** 2011, 100:3000-3007.

**4** Noé F., Doose S., Daidone I., Löllmann M., Sauer M., Chodera J. and Smith J.C. *Dynamical Fingerprints: Understanding biomolecular processes by combination of simulation and kinetic experiments.* **Proc. Natl. Acad. Sci. USA** 2011, 108:4822-4827.

**5** Amadei A., Daidone I., Di Nola A. and Aschi M. *Theoretical-computational modelling of infrared spectra in peptides and proteins: a new frontier for combined theoretical-experimental investigations.* **Curr. Opin. Struct. Biol.** 2010, 20:155-161.

**6** Daidone I.*, Neuweiler H., Doose S., Sauer M. and Smith J.C. *Hydrogen-bond driven loop-closure kinetics in unfolded polypeptide chains*. **PloS Comput. Biol.** 2010, 6(1): e1000645.

**7** Thukral L., Smith J.C.* and Daidone I.* *Common folding mechanism of a β-hairpin peptide via non-native turn formation revealed by unbiased molecular dynamics simulations.* **J. Am. Chem. Soc.** 2009, 131: 18147-18152.

**8** McLain S.E., Soper A.K., Daidone I., Smith J.C. and Watts A. *Charge based interactions between peptides observed as the dominant force for association in aqueous solution.* **Angew. Chem. Int. Ed.** 2008, 47: 9059-9062.

**9** Neusius T., Daidone I., Sokolov I.M. and Smith J.C. *Subdiffusion in peptides originates from fractal-like structure of configuration space.* **Phys. Rev. Lett.** 2008, 100: 188103.

**10** Daidone I., Ulmschneider M., Di Nola A., Amadei A. and Smith J.C. *Dehydration-driven solvent exposure of hydrophobic surfaces as a driving force in peptide folding.* **Proc. Natl. Acad. Sci. USA** 2007, 104:15230-15235.

**11** Daidone I., Amadei A. and Di Nola A. *Theoretical characterization of α-helix and β-hairpin folding kinetics.* **J. Am. Chem. Soc.** 2005, 127:14825-14832.

**12** Daidone I., Amadei A., Roccatano D. and Di Nola A. *Molecular dynamics simulation of protein folding by essential dynamics sampling: folding landscape of horse heart cytochrome c*. **Biophys. J**., 2003, 85:2865-2871.

* corresponding author

## Selected conferences & talks

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| September 2011 | *Seminar: "*XXIV Congresso Nazionale della Società Chimica Italiana", Lecce (Italy) |
| October 2010 | *Invited Speaker*: "Protein folding dynamics: Bridging the gap between theory and experiment", Lausanne (Switzerland) |
| July 2010 | *Invited Speaker:* "2nd Meeting of the Italian and Spanish Crystallographic Associations (MISCA II)", Oviedo (Spain) |
| February 2010 | *Invited Speaker:* "Physics of Protein Folding and Aggregation", Bressanone, (Italy) |
| May 2008 | *Seminar:* EMBIO meeting “Emergent organisation in complex biomolecular systems”, ECLT - Venice (Italy) |
| October 2006 | *Invited Speaker:* Workshop ”Neutron Scattering Highlights on Biological Systems”, |

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| | Taormina (Italy) |
| June 2005 | *Seminar:* RTN meeting “Protein (mis)folding”, Institut Pasteur de Lille (France) |
| March 2005 | *Seminar.* ETH Zurich - RGP *“*Thermodynamic and kinetic characterization of peptide folding by extended molecular dynamics simulations”, Zurich (Switzerland) |
| January 2004 | *Poster:* GRC “Protein folding dynamics”, Ventura, California (USA) |
| June 2003 | *Poster:* PROTEINE 2002 “XVI Meeting of the protein group of the Italian Society of Biochemistry and Molecular Biology”, L’Aquila (Italy) |
| Years 2005-2009 | *Seminar:* Annual workshop on “Methods of Molecular Simulation”, Heidelberg (Germany) |
| Years 2002-2010 | *Seminar:* Annual "Workshop on Molecular theories and simulations”, Gaeta (Italy) |

## Honors and Awards

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| Year 2014 | EU project “fortissimo” within the 7th Framework Programme |
| Year 2010 | Prize: “Enrico Gavuzzo 2008-2009 per ricercatori nel campo del DRUG DESIGN” from the Institute of Crystallography (IC) of the CNR of Bari (Italy) |
| June 2006 | EMBO long term fellowship |
| July 2006 | Marie Curie Intra-European Fellowship |
| August 2006 | DFG Research Grant (Germany) |

## General Skills

*Languages:* Italian, English, Swedish, German

*Programming Languages:* Fortran 77/90, C/C++, awk, html

*Scientific packages:* Gromacs, CHARMM, Matlab, InsightII, GAUSSIAN

*Operating systems:* MS-DOS, Unix/Linux, Windows

*Computer networking:* TCP/IP