PERSONAL INFORMATION

Isabella Daidone

University of l'Aquila (UNIVAQ), Department of Physical and Chemical Sciences (DSFC), via Vetoio-COPPITO 2, 67100, L'Aquila (IT)

+39 0862 433754

isabella.daidone@univaq.it ORCID 0000-0001-8970-8408

https://www.univaq.it/rubrica.php?id=692&docente=on

CURRENT POSITION(S)

Since 05/2015

Associate professor (CHIM03 – Inorganic Chemistry)

Department of Physical and Chemical Sciences of the University of L'Aquila (Italy)

PREVIOUS POSITION(S)

From 01/2009 to 05/2015

Research associate (CHIM03 – Inorganic Chemistry)

Department of Physical and Chemical Sciences of the University of L'Aquila (Italy)

From 06/2007 to 01/2009

Marie Curie fellow (individual fellowship)

"Computational Molecular Biophysics Group" of Prof. Jeremy C. Smith, IWR, Uni Heidelberg (Germany).

From 06/2005 to 05/2007

Post Doctoral fellow

"Computational Molecular Biophysics Group" of Prof. Jeremy C. Smith, IWR, Uni Heidelberg (Germany).

From 11/2004 to 05/2005

Post Doctoral fellow

"*Theoretical and Computational Physical Chemistry Group*" of Prof. Alfredo Di Nola, University of Rome "La Sapienza" (Italy)

EDUCATION AND ACADEMIC DEGREES

From 11/2001 to 10/2004

Ph.D. in Chemistry

Department of Chemistry, University of Rome "La Sapienza" (Italy)

Research project: Study of folding and misfolding processes by the use of computational methods
Supervisors: Prof. Alfredo Di Nola and Prof. Andrea Amadei

From 10/1993 to 05/2001

Degree (Laurea) in Chemistry - Summa cum laude

Department of Chemistry, University of Rome "La Sapienza" (Italy)

Thesis title: Simulazioni di dinamica molecolare del citocromo c. Supervisor: Prof. Alfredo Di Nola

From 10/1993 to 05/2001

High School Diploma (Maturità Scientifica) – 60/60

Liceo scientifico "G.B. Morgagni", Rome (Italy)

ACHIEVEMENTS AND AWARD

Awards

10/04/2017 ASN, Habilitation to Ordinary Professor in Physical Chemistry (sector 03/A2)

12/04/2017 ASN, Habilitation to Ordinary Professor in Inorgnic Chemistry (sector 03/B1)

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)

Grants (last 10 years)

03/2022-present — HE-EIC-Pathfinder Open # 101046424. Title: "Twisted nanophotonic technology for integrated chiroptical sensing of drugs on a chip" (3.600 keuro). Role: Partecipant

07/2020-06/2022 — Grant from UNIVAQ for a 2-years post-doctoral position (50 keuro). Title: A multiscale approach for slow proton transfer reactions in proteins". Role: PI

03/2016-02/2017 — Grant from UNIVAQ for a 1-year post-doctoral position (25 keuro). Title: “Sviluppo di un modello teorico per la bioelettrochimica: applicazioni a celle a biocombustibile”. Role: PI

02/2014-01/2020 — MIUR "SMART Cities and Comunities and Social Innovation”. Title: “Innovazione di prodotto e di processo per una manutenzione, conservazione e restauro sostenibile e programmato del patrimonio culturale” (13.200 keuro). Role: Participant

11/2014-10/2016 — Fortissimo: Factories of the Future Resources, Technology, Infrastructure and Services for Simulation and Modelling - 7th Framework Programme. Title: “Prediction of optical properties of dyes and application for the rational design of time temperature integrators” (250 keuro). Role: Local Coordinator

RELEVANT PUBLICATIONS (last 10 years)

1) Capone M., Sirohiwal A., Aschi M., Pantazis M., Daidone I.
Alternative Fast and Slow Charge-Separation Pathways in Photosystem II.
Angew. Chem., 2023, https://doi.org/10.1002/anie.202216276.

2) Zanetti-Polzi L., Smith M. D., Chipot C., Gumbart J. C., Lynch D. L, Pavlova A., Smith J: C., Daidone. I.
Tuning proton transfer thermodynamics in SARS-CoV-2 main protease: implications for catalysis and inhibitor design. **J. Phys. Chem. Lett.**, 2021, 12: 4195-4202.

3) Biswas A.D., Barone V. and Daidone I.
High Water Density at Non-Ice-Binding Surfaces Contributes to the Hyperactivity of Antifreeze Proteins. **J. Phys. Chem. Lett.**, 2021, 12: 8777-8783.

4) Pavlova A, et al.
Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease.
Chem. Sci., 2021, 12: 1513-1527.

5) Acharya A., et al.
Supercomputer-based ensemble docking drug discovery pipeline with application to COVID-19.
J. Chem. Inf. Model., 2020, 60: 5832-5852.

6) Zanetti-Polzi L., Amadei A, Djemili R., Durot S., Schoepff L., Heitz V., Ventura B., Daidone I.
Allosteric control of naphthalene diimide encapsulation and electron transfer in porphyrin containers: photophysical studies and molecular dynamics simulation. **Chem. Eur. J.**, 2020, 26: 17514-17524.

7) Giliberti V., Polito R., Ritter E., Broser M., Hegemann P., Puskar L., Schade U., Zanetti-Polzi L., Daidone I., Corni S., Rusconi F., Biagioni P., Baldassarre L., Ortolani M.
Tip-Enhanced Infrared Difference-Nanospectroscopy of the Proton Pump Activity of Bacteriorhodopsin in Single Purple Membrane Patches. **Nano Lett.**, 2019, 19: 3104-3114.

8) M. Davis C.M., Zanetti-Polzi L., Gruebele M., Amadei A., Dyer R.B. and Daidone I.
A quantitative connection of experimental and simulated folding landscapes by vibrational spectroscopy. **Chem. Sci.**, 2018, 9: 9002-9011.

9) Zanetti-Polzi, L., Aschi, M., Amadei, A., Daidone, I.
Alternative Electron-Transfer Channels Ensure Ultrafast Deactivation of Light-Induced Excited States in Riboflavin Binding Protein. **J. Phys. Chem. Lett.**, 2017, 8(14), pp. 3321–3327.

10) Zanetti-Polzi L., Daidone I., Bortolotti, C.A and Corni S.
Surface packing determines the redox potential shift of cytochrome c adsorbed on gold.
J. Am. Chem. Soc. 2014, 136: 12929-12937.

11) 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.

12) Daidone I. and Amadei A.
Essential dynamics: foundation and applications.
WIREs Comput. Mol. Sci. 2012, 2:762-770.

ADDITIONAL INFORMATION

Institutional responsibilities

2022/2023 — Member of the evaluation committee of UNIVAQ for the assignment of research grants

From 01/2020–to date — Vice-president of the didactic area council (CAD) in "Scienze e Tecnologie Chimiche e dei Materiali" e in "Scienze Chimiche", UNIVAQ

From 11/2019–to date — Member of the research committee of DSFC, UNIVAQ

Form 07/2019–to date — Member of the Faculty-Students joint committee of DSFC, UNIVAQ

From 2017–to date — University contact person for the coordination of the CISIA entrance tests for the area of Science (TOLC-S)

Member of scientific societies

From 2019 to date — Member of the scientific committee of the "Space-time Multiscale Applications for Research and Technology" Laboratory - SMART, Scuola Normale di Pisa, Italy

From 2020 to date — Member of the scientific board of the “Divisione di chimica teorica e computazionale” of the Italian Society of Chemistry (SCI)

From 2011 to date — Member of the Italian Society of Chemistry (SCI)

Mentorship of students/young researchers/fellows

From 2004 to date — Supervisor of 16 bachelor and master thesis, 6 PhD thesis and 7 post doctoral fellowships.

Claudio Iacobucci is currently employed as a researcher (RTD-B) at UNIVAQ. Roland Schulz is currently employed as HPC Application Engineer for Intel, Hillsboro (USA). Giulia Rossetti is currently employed as Junior Professor at the "Forschungszentrum Jülich", Jülich (Germany). Daniele Narzi is currently employed as a researcher (RTD-A) at UNVAQ. Laura Zanetti-Polzi is currently employed as a researcher ar CNR-NANO (Modena). Lipi Thukral is currently employed as Staff Scientist at CSIR-IGIB, New Delhi (India)

Organisation of conferences/scientific meetings

-07/2023: Psi-K workshop "Principles of light-induced charge transfer for optogenetics”, University of Modena (Italy) - https://psi-k.net/workshops/#

-06/2020: Psi-K workshop "Principles of light-induced charge transfer for optogenetics”, virtual edition - https://optogenetics2021.nano.cnr.it/

-10/2013: “International Workshop on Protein Electron Transfer: from Fundamentals to Applications for Health”, Modena (Italy) - http://www.et4health.unimore.it/site/home.html

-06/2012: Italian Chemistry Society (SCI) conference “TUMA 2012”, Francavilla al Mare (Italy)

-05/2010: "8th Workshop on Molecular theories and simulations”, Gaeta (Italia)
-http://www.dinola.it/html/gaeta/gaeta_locandina_2010.pdf

Invited presentations

-05/2018: “Conference on the Complex Interactions of Light and Biological Matter: Experiments meet Theory”, ICTP, Trieste (Italy)

-10/2010: CECAM workshop "Protein folding dynamics: Bridging the gap between theory and experiment", Lausanne (Switzerland)

-07/2010: "2nd Meeting of the Italian and Spanish Crystallographic Associations (MISCA II)", Oviedo (Spain)

-02/2010: Conference "Physics of Protein Folding and Aggregation", Bressanone (Italy)

-10/2006: Workshop ”Neutron Scattering Highlights on Biological Systems”, Taormina (Italy)

-2002/2005: 1st, 2nd, 3rd and 4th edition of the “Workshop on Molecular theories and simulations”, Gaeta (Italy)

Member of doctoral committees

01/10/2019-to date: PhD program in “Metodi Computazionali e Modelli Matematici per le Scienze e la Finanza”, Scuola Normale Superiore, Pisa (Italy)

01-10-2017-30/09/2019: PhD program in “Methods and Models for Molecuar Sciences”, Scuola Normale Superiore, Pisa (Italy)

01-10-2012- 30-09-2017: PhD program in "Scienze Fisiche e Chimiche", UNIVAQ

01-10-2009-30-09-2012: PhD program in "Chimica per l'ambiente e per i beni culturali" UNIVAQ

Major collaborations

Dr. Laura Zanetti-Polzi, CNR Nano, Modena (Italy)
Prof. Andrea Amadei (Italy)
Prof. Jeremy C. Smith, Oak Ridge National Laboratory - ORNL, Tennesse (USA)
Prof. Greg Scholes, Dept. of Chemistry, Princeton University, Princeton (USA)
Prof. Barbara Ventura, ISOF-CNR, Bologna (Italy)
Prof. Valérie Heitz, LSAMM, University of Strasbourg (France)
Prof. Vincenzo Barone, "Scuola Normale Superiore di Pisa" (Italy)
Prof. Martin Gruebele, “Chemical and Life Sciences Laboratory”, University of Illinois, Urbana Champaign (USA)

Organisational / managerial skills

Currently responsible for a team of 8 people.

Date: 23/02/2023