Sara Del Galdo

25 August 1986, Rome, Italy

Professional Experience:

- January 2022 – Current Position:
  Rtd-A – Science Department, University of Roma Tre, Roma, Italy.
  Supervisor: Prof. B. Capone
  Research Project: "Design of polymeric Smart Materials for selective removal, recovery and re-use of organic and inorganic pollutants from aqueous solutions".

- December 2020 – December 2021:
  Post Doctoral Research Fellow - Physics and Chemistry Department, University of L'Aquila, L'Aquila, Italy.
  Supervisor: Prof. I. Daidone and Prof. C. Casieri
  Research project: "Study on biomass digestion by means of polysaccharide monooxygenases".

- March 2020– December 2020 :
  Visiting Scientist - Chemistry Department, University of Rome Tor Vergata, Roma, Italy.
  Supervisor: Prof. A. Amadei

- March 2019 – February 2020 :
  Post Doctoral Research Fellow - SMART Laboratory, Scuola Normale Superiore, Pisa, Italy.
  Supervisor: Prof. V. Barone
  Research project: "Development and application of multi-scale methods to simulate spectroscopic properties of complex molecular systems".

- March 2018 – February 2019 :
  Post Doctoral Research Fellow - ICCOM, National Research Council, Pisa, Italy & SMART Laboratory, Scuola Normale Superiore, Pisa, Italy.
  Supervisor: Prof. V. Barone and Prof. J. Bloino
  Research project: "Development of methods and algorithms for semiclassical simulation of vibronic spectra".

- February 2017 – February 2018 :
  Post Doctoral Research Fellow - SMART Laboratory, Scuola Normale Superiore, Pisa, Italy.
  Supervisor: Prof. V. Barone
  Research project: "Development of methods and algorithms for analysis of Molecular Dynamics simulations".

Education

2016 *Ph.D. in Chemistry*, Thesis Title: "Unveiling the atomic-molecular behaviour

of complex systems by means of theoretical-computational modelling".
University of Rome Tor Vergata, Rome, Italy. Supervisor: Prof. A. Amadei

2013 *Master Degree* in Chemistry (Laurea Magistrale).
grade: 110/110 cum laude (full honours). Supervisor: Prof. A. Amadei
University of Rome Tor Vergata, Rome, Italy.

2010 *Bachelor Degree* in Chemistry (Laurea Triennale).
grade: 110/110. Supervisor: Prof. L. Stella
University of Rome Tor Vergata, Rome, Italy.

Fellowships, awarded projects, role covered in each project and ability to attract funding

- Winner of RtdA Position at University of Roma Tre, Science Department (FIS03)
- Winner of IST-BRIDGE postdoctoral fellowship at Institute of Science and Technology Austria (ISTA) (December 2021)
- Awarded 3 Italian SuperComputing Resource Allocation – ISCRA project, Application Class C; and 1 Italian SuperComputing Resource Allocation – ISCRA project, Application Class B

Awards

- ECIS Poster Award for the Poster "Addressing the role of hydrophobic interactions to tune thermoresponsiveness in model polymeric systems" (September 2022)

Conferences

- 20/09/2023 " DCTC 2023 - VIII Congresso della Divisione di Chimica Teorica e Computazionale della Società Chimica Italiana"
  Oral contribution: "On the study of thermoresponsive (adsorbent) species at the nanoscale: the case of polyoxazolines"
- 8/09/2023 "The 7th International Soft Matter Conference, ISMC2023", Osaka, Japan.
  Oral Contribution: " Unveiling the thermoresponsive mechanism of PiPOx in aqueous solution".
- 23/06/2023 "Frontiers in Water Biophysics",Ettore Majorana Foundation And Centre For Scientific Culture, Erice (SS), Italy.
  Invited Oral Contribution: "Combined atomistic and coarse-grained approach for the study of thermoresponsive adsorbent species at the nanoscale: the case of polyoxazolines".
- 4-9/09/2022 "ECIS 2022", Chania, Greece.
  Poster: "Addressing the role of hydrophobic interactions to tune thermoresponsiveness in model polymeric systems".

- 02/06/2022 “WaterX@2022 - International Workshop”, La Maddalena (SS), Italy.
  Oral Contribution: “Polymer solubility: the subtle interplay between water-water and polymer-water interactions”.
- 17/09/2021 “SCI2021 XXVII Congresso Nazionale della Società Chimica Italiana”, Online event.
  Oral contribution: “How water density responds to the presence of a crowding agent”.
- 20/09/2019 “DCTC 2019 SESTA EDIZIONE - VI Congresso della Divisione di Chimica Teorica e Computazionale della Società Chimica Italiana”, Arcavacata di Rende (CS), Italia.
  Oral contribution: “Integrated application of variational/perturbative approaches for electronic spectroscopy of complex systems”.
- 5/04/2019 “Young researchers meet molecular spectroscopy”, Pisa (PI), Italia.
  Oral contribution: “Assessment of multi-scale approaches for computing UV-Vis spectra in condensed phases: an effective integration of variational and perturbative QM/MM approaches”.
- 14/02/2019 “2019 Winter Modeling”, Napoli (NA), Italia.
  Invited Oral contribution: “Assessment of multi-scale approaches for computing UV-Vis spectra in condensed phases: toward an effective yet reliable integration of variational and perturbative QM/MM approaches”.
- 5/10/2018 “Problems in discrete dynamics: from biochemical systems to rare events, networks, clustering and related topics IV”, Arcidosso (GR), Italia.
  Oral contribution: “Multiscale approaches for studying spectroscopic properties: the Perturbed Matrix Method”.
- 1/12/2017 “ERC AdG – Barone DREAMS: final meeting”, Pisa (PI), Italia.
  Oral contribution:“Combining Molecular Dynamics and the Perturbed Matrix Method to study Tyrosine UV-Vis spectroscopic properties”.
- 6/10/2017 “Problems in discrete dynamics: from biochemical systems to rare events, networks, clustering and related topics II”, Arcidosso (GR), Italia.
  Oral contribution: “Effects of backbone protonation on Tyrosine UV-VIS absorption spectrum”.
- 24/09/2015 “Tuma XXXIV Convegno delle Sezioni Toscana, Umbria, Marche e Abruzzo della Società Chimica Italiana", Perugia (PG), Italia.
  Oral contribution: “In silico characterization of protein partial molecular volumes and hydration shells”.

Lectures

- 03/2023 – 06/2023 University of Roma Tre, Roma
  Course: Mathematical and Statistical Methods (50 hours)
  Degree Course: Architecture
- 03/2023 – 06/2023 University of Roma Tre, Roma
  Course: Laboratory of Data Analysis for Biology (Exercises) (46 hours)
  Degree Course: Biology
- 09/2022 – 01/2023 University of Roma Tre, Roma
  Course: Physics (Exercises) (20 hours)
  Degree Course: Biology

- 03/2022 – 06/2022 University of Roma Tre, Roma
  Course: Laboratory of Data Analysis for Biology (Exercises) (66 hours)
  Degree Course: Biology
- 24/10/2017 Scuola Normale Superiore, Pisa.
  Lecture:“Theoretical-computational modeling of complex systems beyond the classical limit: the Perturbed Matrix Method” within the course “Frontiere della Chimica”. (1 hour)
- 22/10/2019 Scuola Normale Superiore, Pisa.
  Lecture:“Application of theoretical frameworks to study (bio)chemical phenomena of varying time scales” within the course “Frontiere della Chimica”. (1 hour)

Schools and courses

- 14/02/2023 – 27/02/2023 24th Bologna Winter School, Bioinformatics and Deep learning for biodata analysis [ONLINE]
- 5/10/2020 – 9/10/2020 School on Scientific Data Analytics and Deep Learning @ Cineca [ONLINE] Cineca, Italy.
- 02/2019 – 07/2019 English course - B2.2 level (score: 96/100)
  CLI, Centro Linguistico, University of Pisa, Pisa, Italy
- 09/2018 – 01/2019 English course - B2.1 level
  CLI, Centro Linguistico, University of Pisa, Pisa, Italy

Supervision of Students

- Co-Supervisor of Bachelor Student (Giada Bei).
  AA: 2020-2021
  Thesis Title: “Studio teorico-computazionale per la ricerca degli inibitori della proteasi Mpro del coronavirus SARS-CoV-2” (Theoretical computational study of SARS-CoV-2 Main Protease Inhibitor).
  Physics and Chemistry Department, University of L’Aquila, L’Aquila, Italy.

Skills

Operating System: Linux, Windows.
Programming Languages: Fortran, Python, Bash.
Data Visualization: Matplotlib, Seaborn, Xmgrace.
Data Science: Jupyter, Numpy, Pandas, Scipy, Scikit learn, Xgboost, SQL (basics).
Molecular Modeling: Gromacs, Gaussian, Dalton, MDAnalysis, Joyce.
Molecular Visualization: Molden, VMD, Gaussview.
Text Editor: Vim, LATEX, Microsoft Word.
Languages: Italian (mothertongue), English (fluent), French (scholastic).

List of Publications

1. A Semmeq, S Del Galdo, M Chiarini, I Daidone, C Casieri
   Macromolecular vs molecular crowding in aqueous solutions: A comparative study of PEG400 and ethylene glycol
   J. Mol. Liq. 394, 123713 (2024)
2. CF Vorsmann, S Del Galdo, B Capone, E Locatelli
   Colloidal adsorption in planar polymeric brushes
   Nanoscale Advances 6 (3), 816-825 (2024)
3. S. Del Galdo, C. A. De Filippo, L. Stefanuto, S. Sennato, T. Gasperi, E. Chiessi, B. Capone
   On the nature of the thermoresponsiveness of poly(2-isopropyl-2-oxazoline) in aqueous solution
   J. Mol. Liq. 394, 123713 (2023)
4. A Tripathi, S Del Galdo, B Chandramouli, N Kumar
   Distinct dynamical features of plasmodial and human HSP70-HSP110 highlight the divergence in their chaperone-assisted protein folding
   Biochimica et Biophysica Acta (BBA)-Proteins and Proteomics 1871 (6), 140942 (2023)
5. C. A. De Filippo, S. Del Galdo, P. Corsi, C. De Michele and B. Capone,
   On the role of Polydispersity on the Phase Diagram of Colloidal Solutions
   Soft Matter **19**, 1732, (2023)
6. P. Corsi, C. A. De Filippo, S. Del Galdo and B. Capone
   Unveiling adsorption generality in polymeric macromolecules
   Soft Matter **18**, 6353 (2022)
7. J. Glaser et al
   Hit expansion of a noncovalent SARS-CoV-2 main protease inhibitor
   ACS Pharmacology & Translational Science, 2022, 5(4) 255-265
8. S. Del Galdo, M. Chiarini, C. Casieri and I. Daidone
   High density water clusters observed at high concentrations of the macromolecular crowder PEG400
   J. Mol. Liq. , 2022, 357, 119038
9. S. Del Galdo, M. Aschi and A. Amadei,
   IR spectroscopy of condensed phase systems: Can the environment induce vibrational mode coupling?
   Chem. Phys. Lett., 2021, 763, 1381685
10. G. Mancini, S. Del Galdo, B. Chandramouli, M. Pagliai and V. Barone,
    Computational spectroscopy in solution by integration of variational and perturbative approaches on top of clusterized molecular dynamics.
    J. Chem. Theory Comput., 2020, **16**, 9, 5747–5761
11. S. Del Galdo, M. Fusè and V. Barone,
    CPL Spectra of Camphor Derivatives in Solution by an Integrated QM/MD Approach.
    Front. Chem., 2020, **8**, 584.
12. S. Del Galdo, M. Fusè and V. Barone,
    The ONIOM/PMM Model for Effective Yet Accurate Simulation of Optical and Chiroptical Spectra in Solution: Camphorquinone in Methanol as a Case Study.
    J. Chem. Theory Comput., 2020, **16**, 5, 3294–3306.

13. M. D'Abramo, S. Del Galdo and A. Amadei,
Theoretical–computational modelling of the temperature dependence of the folding–unfolding thermodynamics and kinetics: the case of a Trp-cage.
Phys. Chem. Chem. Phys., *2019*, doi 10.1039/C9CP03303C
14. B. Chandramouli, S. Del Galdo, M. Fusè, V. Barone, G. Mancini,
Two-level stochastic search of low-energy conformers for molecular spectroscopy: implementation and validation of MM and QM models
Phys. Chem. Chem. Phys., *2019*, **21**, 19921-19934
15. L. Zanetti-Polzi, A. D. Biswas, S. Del Galdo, V. Barone, I. Daidone,
Hydration Shell of Antifreeze Proteins: Unveiling the Role of Non-Ice-Binding Surfaces.
J. Phys. Chem. B, 2019, **123** (30), 6474-6480
16. S. Del Galdo, B. Chandramouli, G. Mancini, V. Barone,
Assessment of multi-scale approaches for computing UV-Vis spectra in condensed phases: toward an effective yet reliable integration of variational and perturbative QM/MM approaches.
J. Chem. Theory Comput., 2019, **15** (5), 3170-3184
17. S. Del Galdo, J. Alba, A. Amadei, M. D'Abramo,
Evolutionary Modes in Protein Observable Space: The Case of Thioredoxins.
J. Mol. Evol., 2019, **87**,175-183.
18. B. Chandramouli, S. Del Galdo, G. Mancini, V. Barone,
Mechanistic insights into metal ions transit through threefold ferritin channel.
Biochimica et Biophysica Acta (BBA) - General Subjects, 2019, 1863, 472-480.
19. L. Zanetti-Polzi, S. Del Galdo, I. Daidone, M. D'Abramo, V. Barone, M. Aschi, A. Amadei,
Extending the perturbed matrix method beyond the dipolar approximation: comparison of different levels of theory.
Phys. Chem. Chem. Phys., 2018, **20**, 24369-24378.
20. S. Del Galdo, G. Mancini, I. Daidone, L. Zanetti Polzi, A. Amadei and V. Barone,
Tyrosine absorption spectroscopy: backbone protonation effects on the side chain electronic properties.
J. Comput. Chem., 2018, **39**(22), 1747-1756.
21. B. Chandramouli, S. Del Galdo, G. Mancini, N. Tasinato and V. Barone,
Tailor-made computational protocols for precise characterization of small biological building blocks using QM and MM approaches.
Biopolymers, 2018*,* **109**:e23109.
22. 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.
J. Chem. Theory Comput., 2017, **13**, 5506–5514.
23. A. Amadei, S. Del Galdo and M. D'Abramo,
Density discriminates between thermophilic and mesophilic proteins.
J. Biomol. Struct. Dyn., 2018, **36** (12), 3265-3273
24. S. Del Galdo and A. Amadei,
The unfolding effects on the protein hydration shell and partial molar volume: a

computational study.
Phys. Chem. Chem. Phys., 2016, **18**, 28175–28182.
25. S. Del Galdo, M. Aschi and A. Amadei,
In silico characterization of bimolecular electron transfer reactions: the ferrocene-ferrocenium reaction as a test case.
Int. J. Quantum Chem., 2016, **116**, 1723–1730.
26. S. Del Galdo, P. Marracino, M. D'Abramo and A. Amadei,
In silico characterization of protein partial molecular volumes and hydration shells.
Phys. Chem. Chem. Phys., 2015, **17**, 31270–31277.