Tesi di Dottorato in Fisica:

Computer Simulation of Biological Systems , Anna Battisti (2012) PhD thesis University of Trento, – eprints-phd.biblio.unitn.it
Part1: *Adsorption of DNA oligomers on amine-functionalized surface: insights from computer modeling.* Part2: *Tau, an intrinsically disordered protein*

Lista Delle Pubblicazioni:

Ordered and chaotic dynamics of collective variables in a butane molecule, A. Battisti, R.G. Lalopa, M.D'Alessandro, A. Tenenbaum, Physical Review E **79**, 046206 (2009).

Zeolitic Imidazolate Frameworks for separation of binary mixtures of CO2, CH4 and H2: a computer simulation investigation, A. Battisti, G. Garberoglio and Simone Taioli, Microporous and Mesoporous Materials **143**, 46-53 (2011).

Temperature and solvent dependence of the dynamical landscape of tau protein conformations, Antonio Bianconi, Gabriele Ciasca, Alexander Tenenbaum, Anna Battisti, and Gaetano Campi, Journal of Biological Physics **38**, 169-179 (2011).

Molecular dynamics simulation of intrinsically disordered proteins, Anna Battisti and Alexander Tenenbaum, Molecular Simulation **38,** 139-143 (2012).

Temporary secondary structures in tau, an intrinsically disordered protein, Anna Battisti, Gabriele Ciasca, Alessandro Grottesi , Antonio Bianconi, and Alexander Tenenbaum, Molecular Simulation **38,** 525-533 (2012).

Continuous temperature-induced compaction of the intrinsicall disordered tau protein, G. Ciasca, G. Campi, A. Battisti, G. Rea, P. Pernot, M. Rodio, A. Tenenbaum, and A. Bianconi, Langmuir **28,** 13405-13410 (2012).

Transient tertiary structures in tau, an intrinsically disordered protein. Anna Battisti, Gabriele Ciasca and Alexander Tenenbaum, Molecular Simulation **39**, 1084-1092 (2013).

Self-assembly of mesogenic bent-core DNA nanoduplexes. Khanh Thuy Nguyen, Anna Battisti, Daniele Ancora, Francesco Sciortino and Cristiano De Michele, Soft Matter **11**, 2934-2944 (2014)

Thermal compaction of the intrinsically disordered protein tau: entropic, structural, and hydrophobic factors. Anna Battisti, Gabriele Ciasca, Alessandro Grottesi, and Alexander Tenenbaum, Physical Chemistry Chemical Physics **19,** *8435-8446* (2017).

*Peptide biosensors for anticancer drugs: Design in silico to work in denaturizing environment. Filomena Guida, Anna Battisti, Ivan Gladich, Mauro Buzzo, Elena Marangon, Luciana Giodini, Giuseppe Toffoli, Alessandro Laio, Federico Berti, Biosensors and Bioelectronics **100**, 298-303 (2018)* http://dx.doi.org/10.1016/j.bios.2017.09.012

Toward a unified scoring function for native state discrimination and drug-binding pocket recognition. Anna Battisti, Stefano Zamuner, Edoardo Sarti and Alessandro Laio. *Physical Chemistry Chemical Physics* **20**, 17148-17155 (2018), *DOI: 10.1039/C7CP08170G*

A new design algorithm for selective recognition of anticancer drugs and their metabolites. Anna Battisti, Miguel Soler and Alessandro Laio (in preparation)

Tesi di Dottorato:
Unveiling the atomic-molecular behaviour of complex systems by means of theoretical-computational modelling

Pubblicazioni scientifiche presentate:

1. 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
2. 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.
3. 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
4. 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
5. 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
6. 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
7. 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.
8. 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.
9. 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.
10. 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.

11. 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.
12. 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.

Title of PhD Thesis:
Study of Ionic Liquid–Molecular Liquid Solutions with X-Ray Diffraction, Thermodynamic and Theoretical Methods.

Publications:

A) Publications with peer review process

1. **Salma U.**, Ballirano P., Usula M., Caminiti R., Plechkova N. V., Seddon K. R. and Gontrani L., (2016) "A new insight into the nanostructure of alkylammonium alkanoates based ionic liquids in water", Phys. Chem. Chem. Phys., 18, 11497-11502. (**IF** 2016: 4.449)

2. **Salma U.**, Usula M., Caminiti R., Gontrani L., Plechkova N. V. and Kenneth R. Seddon., (2017) "X- Ray and Molecular Dynamics Studies of Butylammoniu Butanoate- Water Binary Mixtures", Phys. Chem. Chem. Phys., 19, 1975-1981. (**IF** 2017: 4.123)

3. **Salma U**., Plechkova N. V., Caminiti R. and Gontrani L., (2017) "The Opposite Effect of Water and N-Methyl-2-Pyrrolidone Cosolvents on The Nanostructural Organization of Ethylammonium Butanoate Ionic Liquid: a Small and Wide Angle X-Ray Scattering and Molecular Dynamics Simulations Study", J Phys Chem B., 6399-6407. (**IF** 2017: 3.146)

4. Gontrani L., Caminiti R., **Salma U.** and Campetella M., (2017) "A Structural and Theoretical Study of the Alkylammonium Nitrates Forefather: Liquid Methylammonium Nitrate", Chemical Physics Letters, 304-309. (**IF** 2020: 2.328)

B) Publications without peer review process (Conferences)

5. Gontrani L., **Salma U.**, Sadun C., Caminiti R., (2015) "Halogen Bond in Liquid Acetonitriles: the First XRay Diffraction and Molecular Dynamics Study", at Congresso DCTC 2015 (Divisione Chimica Teorica e Computazionale), 12-14 December, CNR, Rome, Italy.

6. **Salma U.**, Caminiti R., and Gontrani L., (2016) "Effect of Water on the Nanostructure of Alkylammonium Based Ionic Liquids", Merck Young Chemists Symposium, October 25th-27th, Rimini, Italy.
7. Gontrani L., **Salma U.** and Caminiti R., (2017) "To swell or to shrink? Alkylammonium alkanoates plus molecular solvents." 10-14 September, 2017, Paestum, Italy.

Publication List

Publications

1. *Constrained dynamics of maximally entangled bipartite system*, A. Bashir & **M. A. Wasay**. **Eur.Phys.J.C 81, 4 no.303 (2021)**.
2. *Multichannel asymmetric transmission through a dimer defect with saturable inter-site nonlinearity*, **M. A. Wasay** & M. Johansson. **J.Phys.A: Math.Theor.(53) 395702 (2020)**. e-print:arXiv:2003.05963
3. *Geometric description of Schrödinger equation in Finsler and Funk geometry*, A. Bashir, B. Koch, **M. A. Wasay**. **Int.J.Geom.Meth.Mod.Phys.16 no.7, 1950098 (2019)**. e-print:arXiv:1904.12153
4. *Enhanced nonreciprocal transmission through a saturable cubic-quintic nonlinear dimer defect*, **M. A. Wasay**, Marcelo I.Lyra & Byoung S.Ham **Scientific Reports (9) 1871 (2019)**. e-print:arXiv:1901.05224
5. *Asymmetric wave transmission through one dimensional lattices with cubic-quintic nonlinearity*, **M. A. Wasay**. **Scientific Reports (8) 5987 (2018)**. e-print:arXiv:1810.00631
6. *Nonreciprocal wave transmission through an extended discrete nonlinear Schrödinger dimer*, **M. A. Wasay**. **Phys.Rev.E 96 (5), 052218 (2017)**.
7. *Geometric description of Schrödinger equation in* $3n+1$ *dimensional configuration space*, **M.A. Wasay**, A. Bashir, B. Koch, A. Ghaffar **Int.J.Geom.Meth.Mod.Phys. 14, 10 1750149 (2017)**. e-print:arXiv:1703.09901
8. *Two particle entanglement and its geometric duals*, **M.A. Wasay** & A. Bashir. **Eur.Phys.J.C 77, 12 no.820 (2017)**. e-print:arXiv:1708.03164
9. *Supersymmetric quantum mechanics and topology*, **M. A. Wasay**, **Adv.High Energy Phys. 2016, 3906746 (2016)**. e-print:arXiv:1603.07691
10. *An inconsistency in the spectrum of bosonic open 2-brane*, **M. A. Wasay** & D.f. Zeng, **Adv.High Energy Phys. 2015, 360356 (2015)** e-print:arXiv:1510.02414
11. *Quantization and spectrum of RNS supersymmetric open 2-brane*, **M. A. Wasay**, Y.C. Huang, D.f. Zeng, **Nucl.Phys.B 892, 353 (2015)**.
12. *Spectrum of supersymmetric and bosonic open 2-branes*, **M. A. Wasay**, Mathematical Physics: Proceedings of the 14th Regional Conference. World Scientific Singapore, (2018). ISBN: 978-981-3224-97-1 e-print:arXiv:1704.04210
13. *Supersymmetric open 2-branes and Nonlinear Schrödinger Equation*, by **M. A. Wasay**, PhD Thesis.

Europass Curriculum Vitae

Personal information

First name(s) / Surname(s)	
Address	
Telephone(s)	
E-mail(s)	
Nationality	
Date of birth	
Gender	

Desired employment / Occupational field

Physicist, Theoretical and Computational Biophysics

Work experience

Dates	01/01/2007 - Present
Occupation or position held	Research Collaboration
Main activities and responsibilities	*Modeling and simulation of Intrinsically Disordered Proteins*
Name and address of employer	Prof. Alexander Tenenbaum Piazzale A. Moro 5, 00185 Rome (Italy)

Dates	01/04/2019 - 31/03/2020
Occupation or position held	Post-Doctoral Research
Main activities and responsibilities	Investigation of liquid intrusion in porous materials via continuum rare event simulation techniques.
Name and address of employer	Prof. Simone Meloni University of Rome “La Sapienza” Dipartimento di Ingegneria Meccanica e Aereospaziale.

Dates	01/12/2014 - 30/11/2017
Occupation or position held	Post-Doctoral Research
Main activities and responsibilities	*Design of peptides capable of binding to drugs and tumor markers and development of a new scoring function for protein folding and drug-binding pocket recognition.*
Name and address of employer	Prof. Alessandro Laio Scuola Internazionale Superiore di Studi Avanzati (SISSA), Via Bonomea 265, I-34136 Trieste, Italy

Dates	17/04/2012 - Present
Occupation or position held	European Commission (EC) Project Review Expert
Main activities and responsibilities	*Review of European Project.*
Name and address of employe	European Commision
Expert number	EX2013D133810
Dates	01/05/2013 - 30/04/2014
Occupation or position held	Post-Doctoral Position
Main activities and responsibilities	*Full-atom simulations of the DNA's end-to-end aggregation and formation of β-lactoglobulin fibrils.*
Name and address of employer	Prof. Francesco Sciortino University of Roma “La Sapienza”, Department of Physics
Dates	01/03/12 - 31/12/2013
Occupation or position held	Research Collaboration
Main activities and responsibilities	*Modeling and Molecular Dynamics Simulations of Biological Systems.*
Name and address of employer	Prof. Maurizio Dapor Interdisciplinary Laboratory for Computational Science (LISC) via Sommarive, 18 38123 Trento (Italy)
Dates	15/02/2010 - 28/05/2010
Occupation or position held	Teaching Assistant
Main activities and responsibilities	*Teaching assistant for the Course of Many Body Theory.*
Name and address of employer	University of Trento via Verdi,6 38100 Trento
Dates	01/08/2008 - 30/10/2008
Occupation or position held	Research with scholarship
Main activities and responsibilities	*Development of a program to calculate the coherence time in the dynamics of biomolecules.*
Name and address of employer	Prof. Alexander Tenenbaum Piazzale A. Moro 5, 00185 Rome (Italy)

Education and training

Dates	24/02/12
Title of qualification awarded	PhD in Physics
Principal subjects / occupational skills covered	*Modeling and Computer Simulations of Biological Systems*
Name and type of organisation providing education and training	University of Trento (University) via Sommarive 18, 38123 Trento (Italy)
Level in national or international classification	Doctoral School

Dates	13/12/07
Title of qualification awarded	Master's Degree in Physisc (Vecchio Ordinameto) 110/110
Principal subjects / occupational skills covered	*Ordered and chaotic dynamics of collective variables in a butane molecule.*
Name and type of organisation providing education and training	University of Roma "La Sapienza" (University) Piazzale A. Moro 5, 00185 Roma (Italy)
Level in national or international classification	University
Dates	02/12/2013 - 05/12/2013
Title of qualification awarded	Certificate of Attendance
Subjects	Workshop DNA-based self-assembly: theory, simulations and experiments
Name and type of organisation providing education and training	DaCAM Danube Center for Atomistic Modelling
Dates	15/09/2013 - 19/09/2013
Title of qualification awarded	Certificate of Attendance
Subjects	International Soft Matter Conference 2013
Name and type of organisation providing education and training	University of Rome “La Sapienza”
Dates	22/02/2011 - 24/02/2011
Title of qualification awarded	Certificate of Attendance
Subjects	Classical Molecular Dynamics Simulations for biological systems
Name and type of organisation providing education and training	CASPUR Consorzio Interuniversitario per le Applicazioni di Supercalcolo per Univesità e Ricerca
Dates	15/12/2009 - 17/12/2009
Title of qualification awarded	Certificate of Attendance
Subjects	Scientific and technical calculation in fortran 95
Name and type of organisation providing education and training	CASPUR Consorzio Interuniversitario per le Applicazioni di Supercalcolo per Univesità e Ricerca
Dates	06/07/2009 - 10/07/2009
Title of qualification awarded	Certificate of Attendance
Subjects	Linking Nuclei, Molecules and Condensed Matter: Computational Quantum Many-Body Approaches
Name and type of organisation providing education and training	ETC* European Center for Theoretical Studies in Nuclear Physics and related Areas
Dates	06/07/2008 - 15/07/2008
Title of qualification awarded	Certificate of Attendance
Subjects	Methods in Molecular Simulation Summer School
Name and type of organisation providing education and training	University of Sheffield and Sheffield Hallam University

Personal skills and competences

Other language(s)

Self-assessment	Understanding				Speaking				Writing	
European level (*)	Listening		Reading		Spoken interaction		Spoken production			
English	B2	Independent user	B2	Independent user	B2	Independent user	B2	Independent user	B2	Independent user
French	A1	Basic User	A1	Basic User	A1	Basic User	A1	Basic User	A1	Basic User

(*) Common European Framework of Reference (CEF) level

Social skills and competences

Organisational skills and competences: Positive and optimistic approach to activities, people, events. Ease and enjoyment working with other cultures.

Technical skills and competences: High Performance Computation, Modeling, Molecular Dynamics Simulations.

Computer skills and competences: Linux, Gromacs, Amber, LateX, Fortran, Matlab 7.0, Maple, Xmgrace, gnuplot, VMD, plumed, shell.

Driving licence(s): A1, B

Publications:

Ordered and chaotic dynamics of collective variables in a butane molecule, A. Battisti, R.G. Lalopa, M.D'Alessandro, A. Tenenbaum, Physical Review E **79**, 046206 (2009).

Zeolitic Imidazolate Frameworks for separation of binary mixtures of CO2, CH4 and H2: a computer simulation investigation, A. Battisti, G. Garberoglio and Simone Taioli, Microporous and Mesoporous Materials **143**, 46-53 (2011).

Temperature and solvent dependence of the dynamical landscape of tau protein conformations, Antonio Bianconi, Gabriele Ciasca, Alexander Tenenbaum, Anna Battisti, and Gaetano Campi, Journal of Biological Physics **38**, 169-179 (2011).

Molecular dynamics simulation of intrinsically disordered proteins, Anna Battisti and Alexander Tenenbaum, Molecular Simulation **38,** 139-143 (2012).

Temporary secondary structures in tau, an intrinsically disordered protein, Anna Battisti, Gabriele Ciasca, Alessandro Grottesi , Antonio Bianconi, and Alexander Tenenbaum, Molecular Simulation **38,** 525-533 (2012).

Continuous temperature-induced compaction of the intrinsicall disordered tau protein, G. Ciasca, G. Campi, A. Battisti, G. Rea, P. Pernot, M. Rodio, A. Tenenbaum, and A. Bianconi, Langmuir **28,** 13405-13410 (2012).

Computer Simulation of Biological Systems , Anna Battisti (2012) PhD thesis University of Trento, – eprints-phd.biblio.unitn.it Part1: *Adsorption of DNA oligomers on amine-functionalized surface: insights from computer modeling.* Part2: *Tau, an intrinsically disordered protein*

Transient tertiary structures in tau, an intrinsically disordered protein. Anna Battisti, Gabriele Ciasca and Alexander Tenenbaum, Molecular Simulation **39**, 1084-1092 (2013).

Self-assembly of mesogenic bent-core DNA nanoduplexes. Khanh Thuy Nguyen, Anna Battisti, Daniele Ancora, Francesco Sciortino and Cristiano De Michele, Soft Matter **11**, 2934-2944 (2014)

Thermal compaction of the intrinsically disordered protein tau: entropic, structural, and hydrophobic factors. Anna Battisti, Gabriele Ciasca, Alessandro Grottesi, and Alexander Tenenbaum, Physical Chemistry Chemical Physics **19,** *8435-8446* (2017).

Peptide biosensors for anticancer drugs: Design in silico to work in denaturizing environment. Filomena Guida, Anna Battisti, Ivan Gladich, Mauro Buzzo, Elena Marangon, Luciana Giodini, Giuseppe Toffoli, Alessandro Laio, Federico Berti, Biosensors and Bioelectronics ***100****, 298-303 (2018)* http://dx.doi.org/10.1016/j.bios.2017.09.012

Toward a unified scoring function for native state discrimination and drug-binding pocket recognition. Anna Battisti, Stefano Zamuner, Edoardo Sarti and Alessandro Laio. *Physical Chemistry Chemical Physics* **20**, 17148-17155 (2018), *DOI: 10.1039/C7CP08170G*

A new design algorithm for selective recognition of anticancer drugs and their metabolites. Anna Battisti, Miguel Soler and Alessandro Laio (in preparation)

CURRICULUM VITAE

Sara Del Galdo

SUMMARY
I am a theoretical-computational chemist with a research background in molecular mechanics, quantum mechanics and multi-scale procedures.
Over the years, I developed an expertise in Molecular Dynamics (MD) simulations and analyses. I worked on the implementation of a theoretical model (named as PMM) within a quantum-mechanical calculation software.
I recently developed an interest towards Machine Learning (both supervised and unsupervised techniques), that I applied to analyze MD results.
I co-authored around 18 scientific articles and presented my results in several conferences.
I gave seminars for masters students in Scuola Normale Superiore, Pisa.

PROFESSIONAL EXPERIENCES

Date	1/12/2020 – Current Position
Research Group and Institution	Physics and Chemistry Department, Prof I Daidone, Prof. C. Casieri. University of L'Aquila, L'Aquila, Italy.
Position	Post Doctoral Research Fellow on the Research Project: "SMARTCITIES". Research Project: "Study on biomass digestion by means of polysaccharide monooxygenases"
Date	1/03/2020 – 30/11/2020
Research Group and Institution	Theoretical and Computational Physical Chemistry group, Prof A. Amadei. University of Rome Tor Vergata, Rome, Italy.
Position	Scientific collaborator
Date	1/03/2019 – 29/02/2020
Research Group and Institution	SMART Laboratory, Prof V. Barone. Scuola Normale Superiore, Pisa, Italy.
Position	Post Doctoral Research Fellow on the Research Project: "Development and application of multi-scale methods to simulate spectroscopic properties of complex molecular systems".

Date	15/03/2018 – 28/02/2019
Research Group and Institution	SMART Laboratory, Prof V. Barone, Prof. J. Bloino. Consiglio Nazionale delle Ricerche di Pisa - Istituto di Chimica dei Composti OrganoMetallici.
Position	Post Doctoral Research Fellow on the Project PRIN 2015 - Computational protocols to simulate optical, vibrational and vibronic responses of medium-to-large systems" and "SMODATA - Sviluppo di MODelli per i mATeriali avanzati e l'energiA", Research Project: "Development of methods and algorithms for semiclassical simulation of vibronic spectra".
Date	20/02/2017-19/02/2018
Research Group and Institution	SMART Laboratory, Prof V. Barone. Scuola Normale Superiore, Pisa, Italy.
Position	Post Doctoral Research Fellow on the ERC AdG Project "Development of a Research Environment for Advanced Modelling of Soft Matter", Research Project: "Development of methods and algorithms for analysis of Molecular Dynamics simulations".

EDUCATION

Date	07/02/2017
Institute	University of Rome Tor Vergata, Rome, Italy.
Qualification	Philosophiae Doctor in Chemistry. PhD Thesis title: "*Unveiling the atomic-molecular behaviour of complex systems by means of theoretical-computational modelling*". Supervisor: Dr. A. Amadei.
Date	10/07/2013
Institute	University of Rome Tor Vergata, Rome, Italy.
Qualification	Master Degree in Chemistry. Thesis title:"*Theoretical study of unfolding-folding process of peptides and proteins*". Supervisor: Dr. A. Amadei. Mark: 110/110 cum laude.
Date	30/09/2010
Institute	University of Rome Tor Vergata, Rome, Italy.

Qualification	Bachelor Degree in Chemistry. Thesis title: "*Spectroscopic study of the role of Proline on the activity and selectivity of an antimicrobial peptide"*. Supervisor: Prof. L. Stella. Mark: 110/110.
Date	July 2005
Institute	Liceo Ginnasio Statale Immanuel Kant, Rome, Italy.
Qualification	Literature based high school certificate. Mark: 90/100.

PUBLICATIONS

- S. Del Galdo, M. Chiarini, C. Casieri and I. Daidone
  What happens to water in crowded environments?
  (Manuscript in preparation)
- 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
- 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
- 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.
- 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.
- 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
- 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
- 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
- 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

- 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.
- 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.
- 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.
- 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.
- 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.
- 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.
- 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
- 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.
- 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.
- 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.

CONFERENCES

- 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.
  Oral contribution as invited speaker: “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”.

SCHOOLS

- 5/10/2020 – 9/10/2020 Cineca, Roma.
  [ONLINE] School on Scientific Data Analytics and Deep Learning @ Cineca

LECTURES AND SEMINARS

- 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”.
- 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”.

GENERAL SKILLS

Languages: Italian (mother tongue), English (Upper Intermediate), French (Scholastic).

Operating systems: Unix/Linux, Windows
Programming Languages: Fortran, Bash, Python.
Data Visualization: Matplotlib, Xmgrace, Seaborn
Data Science: Numpy, Pandas, Jupyter, Scipy, ScikitLearn, xgboost, SQL (basics)
Scientific packages: Gromacs, Joyce, VMD, Molden, GAUSSIAN, Dalton , MD Analysis.

Curriculum Vitae

Umme Salma

Educational Career

Degree	**Doctor of Philosophy (PhD)**
Major	Physical Chemistry
Session	2014-2017
University/Institute	"La Sapienza" University of Rome, Rome (Italy)
Thesis Title	Study of Ionic Liquid–Molecular Liquid Solutions with X-Ray Diffraction, Thermodynamic and Theoretical Methods

Degree	**Master of Philosophy (MPhil)**
Major	Physical Chemistry
Session	2011-2013
University/Institute	University of Sargodha, Sargodha (Pakistan)
Thesis Title	A Theoretical (DFT) Study on the Second-Order Nonlinear Optical Response of Push-Pull Derivatives of Porphyrin
Main Courses	Physical Chemistry of High Polymers, Advanced Chemical Kinetics, Surface Chemistry, Solution Chemistry, Photochemistry

Degree	**Master of Science (MSc)**
Major	Chemistry
Session	2008-2010
University/Institute	University of Punjab, Lahore (Pakistan)
Main Courses	Physical Chemistry, Organic Chemistry, inorganic Chemistry, Applied Chemistry

Degree	**Bachelors of Science (BSc)**
Major	Chemistry, Zoology, Botany
Session	2006-2008
University/Institute	University of Sargodha, Sargodha (Pakistan)

Professional Degree (Teaching)	**Bachelors of Education (B.Ed.)**
Major	Leadership and Management, Educational Technology and Evaluation, Teacher Education, Science Education
Session	2013-2014
University/Institute	Allama Iqbal Open University, Islamabad (Pakistan)

Research Interests	• Computational/theoretical chemistry, modelling the complex molecular systems, molecular simulations, Ab initio methods (HF/DFT). • Synthesis and characterization of ionic liquid, deep eutectic solvents and polymeric materials using X-Ray and neutron scattering (SAXS and WAXS), spectroscopic measurements and applications of ionic liquids

	in drugs designing and ionic liquids-mixtures in electrochemistry, surface chemistry, catalysis, energy production, as green solvents and in pharmaceutical technology.
Teaching Experience	• Lecturer of Chemistry and academic coordinator at Punjab College Sargodha from May 2012 to Oct. 2014. • Lecturer of Chemistry at ITM College of Science and Technology, Sargodha from September 2010 to April 2012.
Research Experience	• Research experience as a **Research Associate** of three months at The Queen's University of Belfast, UK
Awards & Prizes	• Winner of international scholarship from "La Sapienza" University of Rome, Italy. (Rank-1) • Winner of PhD MOBILITY FELLOWSHIP 2016 "La Sapienza" University of Rome, Italy. • Winner of merit scholarship during M.Sc. from University of Punjab, Lahore (Pakistan). • The prize was warded with "Best Teacher Award" from Punjab College of Science, Sargodha. • Was selected as a "Teachers Trainer" to deliver the lectures on teaching methods and classroom environment.
Computer Skills	• AMBER • GROMACS • Gaussain • VMD • TRAVIS • Microsoft Office • LINUX

Publications	• U. Salma et al., "A new insight into the nanostructure of alkylammonium alkanoates based ionic liquids in water", *Phys. Chem. Chem. Phys.,* 2016, 18, 11497-11502. • U. Salma et al., "X-Ray and Molecular Dynamics Studies of Butylammonium Butanoate-Water Binary Mixtures", *Phys. Chem. Chem. Phys* 2017, 19, 1975-1981. • U. Salma et al., "The Opposite Effect of Water and N-Methyl-2-Pyrrolidone Cosolvents on The Nanostructural Organization of Ethylammonium Butanoate Ionic Liquid: a Small and Wide Angle X-Ray Scattering and Molecular Dynamics Simulations Study", *J Phys Chem B.*, 2017, 6399–6407. • U. Salma et al., "A Structural and Theoretical Study of the Alkylammonium Nitrates Forefather: Liquid Methylammonium Nitrate", *Chemical Physics Letters*, 2017, 304-309. • L. Gontrani, U. Salma, C. Sadun, R. Caminiti, "Halogen Bond in Liquid Acetonitriles: the First X-Ray Diffraction and Molecular Dynamics Study", at *Congresso DCTC 2015 (Divisione Chimica Teorica e Computazionale),* 12-14 December, 2015, CNR, Rome, Italy.

	• U. Salma, R. Caminiti and L. Gontrani, "Effect of Water on the Nanostructure of Alkylammonium Based Ionic Liquids", *Merck Young Chemists Symposium*, October 25th-27th, 2016 Rimini, Italy. • Lorenzo Gontrani, Umme Salma and Ruggero Caminiti, "To swell or to Shrink? Alkylammonium alkanoates plus molecular solvents." 10-14 September, 2017, Paestum, Italy.

Professional Skills and Abilities	• Considerable Leadership, Management and Research Skills • Ability to demonstrate knowledge and understanding of essential facts, concepts, principles, and theories relating to the subject areas. • Ability to apply such knowledge and understanding to the solution of problems mostly of familiar nature. • Skills in the evaluation, interpretation and synthesis of chemical information data. • Skills in communication scientific materials and arguments.

DR. MUHAMMAD ABDUL WASAY

Personal

Education & Training

Postdoctoral Research Associate
Gwangju Institute of Science & Technology,
Gwangju, South Korea.
April 2018 - March 2019

PhD. Physics
Institute of Theoretical Physics,
Beijing University of Technology, Beijing, China.
Graduated: July, 2015

M.S. Physics
Uppsala University, Uppsala, Sweden.
Graduated: March, 2010

MSc. Mathematics
Quaid-i-Azam University, Islamabad, Pakistan.
Graduated: June, 2006

Experience

1. **Assistant Professor of Physics** **September 2015 - To date**
   University of Agriculture, Faisalabad, Pakistan.
2. **Teaching & Research Assistant** **May 2010 - June 2011**
   Department of Physics, LUMS SSE, Lahore, Pakistan.

Courses Taught

1. Methods of Mathematical Physics (MPhil)
2. Mathematical Physics I&II (MSc)
3. Quantum Mechanics I&II (MSc)
4. Advanced Quantum Mechanics (MPhil)
5. Classical Mechanics (MSc)

6. Chaos & Nonlinear Phenomena (unofficially taught to research students)
7. String Theory (unofficially taught to research student)
8. Quantum Field Theory (unofficially taught to research student)

Visiting Research Fellowship

1. Visiting Research Fellowship funded by the *IBS Center for Theoretical Physics of Complex Systems*, South Korea: 10-2016 To 11-2016.

International Conferences as Speaker

1. 14th Regional conference on Mathematical Physics, November 9-14, 2015, Quaid-i-Azam University, Islamabad.
(Gave a talk: Spectrum of supersymmetric and bosonic open 2-branes)

Seminars Given

1. *Enhanced nonreciprocal transmission via nonlinear dimer defects*, given at PIP Center G.I.S.T, Gwangju, South Korea. February, 2019.
2. *An extended DNLS model as a wave diode*, given at IBS Center for Theoretical Physics of Complex systems, Daejeon, South Korea. October, 2016.
3. *Gravitational waves*, given at Physics department, Univ. of Agriculture, Faisalabad, March, 2016.
4. *Supersymmetric Quantum Mechanics and the Topological Index*, given at Institute of Theoretical Physics, BJUT, Beijing, October, 2011.
5. *Spectrum issues in bosonic open branes*, given at Institute of Theoretical Physics, BJUT, Beijing, February, 2015.

Student Supervision

Number of MSc students having completed their report: 41
Number of Mphil research students having completed their thesis: 06
Number of Mphil research students currently in supervision (2021 grad.): 14
Number of PhD students in supervision: 01

Journal Publications

1. *Constrained dynamics of maximally entangled bipartite system*, A. Bashir & **M. A. Wasay**. **Eur.Phys.J.C 81, 4 no.303 (2021)**.
(Corresponding author)

2. *Multichannel asymmetric transmission through a dimer defect with saturable inter-site nonlinearity*, **M. A. Wasay** & M. Johansson. **J.Phys.A: Math.Theor.(53) 395702 (2020)**. e-print:arXiv:2003.05963
(Corresponding & First author)
3. *Geometric description of Schrödinger equation in Finsler and Funk geometry*, A. Bashir, B. Koch, **M. A. Wasay**. **Int.J.Geom.Meth.Mod.Phys.16 no.7, 1950098 (2019)**. e-print:arXiv:1904.12153
(Corresponding author)
4. *Enhanced nonreciprocal transmission through a saturable cubic-quintic nonlinear dimer defect*, **M. A. Wasay**, Marcelo L.Lyra & Byoung S.Ham **Scientific Reports (9) 1871 (2019)**.(Nature Publishing Group)
e-print:arXiv:1901.05224
(Corresponding & First author)
5. *Asymmetric wave transmission through one dimensional lattices with cubic-quintic nonlinearity*, **M. A. Wasay**, **Scientific Reports (8) 5987 (2018)**. (Nature Publishing Group) e-print:arXiv:1810.00631
(Solo author)
6. *Nonreciprocal wave transmission through an extended discrete nonlinear Schrödinger dimer*, **M. A. Wasay**. **Phys.Rev.E 96 (5), 052218 (2017)**. (American Physical Society)
(Solo author)
7. *Geometric description of Schrödinger equation in* $3n+1$ *dimensional configuration space*, **M.A. Wasay**, A. Bashir, B. Koch, A. Ghaffar **Int.J.Geom.Meth.Mod.Phys. 14, 10 1750149 (2017)**.
e-print:arXiv:1703.09901
(Corresponding & First author)
8. *Two particle entanglement and its geometric duals*, **M.A. Wasay** & A. Bashir. **Eur.Phys.J.C 77, 12 no.820 (2017)**. e-print:arXiv:1708.03164
(Corresponding & First author)
9. *Supersymmetric quantum mechanics and topology*, **M. A. Wasay**, **Adv.High Energy Phys. 2016, 3906746 (2016)**. e-print:arXiv:1603.07691
(Solo author)
10. *An inconsistency in the spectrum of bosonic open 2-brane*, **M. A. Wasay** & D.f. Zeng, **Adv.High Energy Phys. 2015, 360356 (2015)**
e-print:arXiv:1510.02414
(Corresponding & First author)
11. *Quantization and spectrum of RNS supersymmetric open 2-brane*, **M. A. Wasay**, Y.C. Huang, D.f. Zeng, **Nucl.Phys.B 892, 353 (2015)**.
(Corresponding & First author)

Computational Skills	My approach in research is mostly analytical and computational and I am well versed in technical computing using MATLAB, Mathematica and Python.

Publications in International Conference Proceedings	1. *Spectrum of supersymmetric and bosonic open 2-branes*, **M. A. Wasay**, Mathematical Physics: Proceedings of the 14th Regional Conference. World Scientific Singapore, (2018). ISBN: 978-981-3224-97-1 e-print:arXiv:1704.04210 (Solo author)

Paper(s) In Preperation	1. "Nonrecirpocal transmission through discrete nonlinear quadratic-cubic structures", **M. A. Wasay** (In Preperation).
