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Alessandra Savarese

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WORK EXPERIENCE

Alma Mater Studiorum - University of Bologna – Bologna, Italy

Address: Via Piero Gobetti 85, 40129 Bologna (Italy) | **Name of unit or department:** Department of Chemistry "Giacomo Ciamician"

University research assistant

[01/05/2025 – 31/10/2025]

RESEARCH FELLOWSHIP: Computational study on polycyclic aromatic hydrocarbons (PAHs) growth
Research Group: Rotational and Computational Spectroscopy Laboratory
Supervisor: Prof. Cristina Puzzarini
Project: "SMART_H2 - Simulations, modeling and applications of plasma-assisted conversion of methane to hydrogen and carbon"

EDUCATION AND TRAINING

Master's Degree in Chemistry (curriculum Physical Chemistry)

University of Pisa [09/2019 – 12/2022]

Address: Via Giuseppe Moruzzi 13, 56124 Pisa (Italy) | **Field(s) of study:** Natural sciences, mathematics and statistics: • Chemistry | **Final grade:** 110/110 cum Laude | **Level in EQF:** EQF level 7 | **Type of credits:** CFU | **Number of credits:** 120 | **Thesis:** "The Minimum Energy Principle Applied to the $C_3H_6O_2$ Isomer Family: Identification and Spectral Characterization of the Best Candidates for Radioastronomical Detection". Supervisors: Prof. Filippo Lipparini, Prof. Cristina Puzzarini.

MASTER'S DEGREE RESEARCH INTERNSHIP: Computational and experimental rotational spectroscopy applied to astrochemistry
Alma Mater Studiorum - University of Bologna, Department of Chemistry "Giacomo Ciamician"
06/2024-03/2025
Research Group: Rotational and Computational Spectroscopy Laboratory
Supervisor: Prof. Cristina Puzzarini

- Employed a computation protocol based on the minimum energy principle to gauge the energetic stability of the members of the $C_3H_6O_2$ isomer family, with the aim of identifying the best candidates for radioastronomical detection within the family. This energetic investigation was conducted by means of increasingly accurate calculations employing Density Functional Theory and composite schemes rooted in Coupled-Cluster theory.
- Attempted to record the experimental rotational spectrum in the 80-120 GHz frequency range of 3-hydroxypropanal (unstable, non-commercial) through its *in situ* production. This was done with the aid of a simulated spectrum of 3-hydroxypropanal obtained through theoretically predicted spectroscopic parameters.
- Recorded and analyzed the experimental rotational spectrum of glycidol (stable, commercial sample) in the 65-120 GHz, 146-330 GHz, and 440-520 GHz frequency ranges, thus obtaining a new and improved set of spectroscopic parameters for its two most stable conformers.

MASTER'S DEGREE RESEARCH INTERNSHIP: Cholesky decomposition implementation of the perturbative triple excitations' correction to the Coupled-Cluster with single and double excitations energy

University of Pisa, Department of Chemistry and Industrial Chemistry
03/2024-06/2024
Research Group: MoLECoLab
Supervisor: Prof. Filippo Lipparini

- Implemented the perturbative triple excitations (T) correction to the Coupled-Cluster with single and double excitations (CCSD) energy, employing the Cholesky Decomposition of the two-electron repulsion integrals (ERIs) matrix. This was done in a development version of the CFOUR suite of programs, employing the Fortran 90 programming language.
- Goals achieved through this preliminary implementation: removal of the need for an initial transformation of the ERIs matrix from the atomic orbitals basis to the molecular orbitals basis, and reduction of the memory storage requirements for the ERIs. This makes the present implementation more suitable for the description of medium-sized systems, with respect to the classical implementation.

RELEVANT COURSEWORK:

- Chemical-Physical Methods for Atmospheric Chemistry and Astrochemistry
- Advanced Spectroscopic Methods
- Biophysical Chemistry
- Theoretical Chemistry
- Quantum Chemistry and Molecular Modeling
- Statistical Thermodynamics
- Photochemistry: Theory and Simulation Methods

Bachelor's Degree in Chemistry

University of Pisa [09/2019 – 12/2022]

Address: Via Giuseppe Moruzzi 13, 56124 Pisa (Italy) | **Field(s) of study:** Natural sciences, mathematics and statistics: ● Chemistry | **Final grade:** 110/110 cum Laude | **Level in EQF:** EQF level 6 | **Type of credits:** CFU | **Number of credits:** 180 | **Thesis:** "Characterization of 1D Coordination Polymers by Means of Solid State NMR Spectroscopy". Supervisor: Prof. Marco Geppi.

BACHELOR'S DEGREE RESEARCH INTERNSHIP: Characterization of Hg(II)-bispidine 1D Coordination Polymers by means of Solid State NMR Spectroscopy
09/2022 - 12/2022
University of Pisa, Department of Chemistry and Industrial Chemistry
Research group: SolStiCE
Supervisor: Prof. Marco Geppi

- Exploited Solid State NMR (SSNMR) spectroscopy to study Hg(II)-bispidine 1D coordination polymers characterized by two different topologies (zig-zag, polycatenane) and by solvent molecules (chlorobenzene) trapped inside their structures.
- Recorded ^{1}H, ^{13}C and ^{199}Hg high-resolution SSNMR spectra of the aforementioned coordination polymers, and measured their T_1 and T_2 spin-relaxation times by means of temperature-controlled low-resolution SSNMR experiments.
- Analyzed the aforementioned spectra in order to characterize the Hg(II)-bispidine 1D coordination polymers in terms of their dynamics and mobility, with the final aim of understanding their adsorption and separation properties.

RELEVANT COURSEWORK:

- Physical Chemistry II and Laboratory: Quantum Mechanics, Spectroscopy, Molecular Modeling
- Photochemistry: Phenomenological Aspects
- Atmospheric Chemistry
- Errors and Data Analysis
- Complements of Mathematics for Chemists

High School Diploma in Classical Studies

Cornelio Tacito High School [09/2014 – 07/2019]

Address: Via Giordano Bruno 4, 00195 Roma (Italy) | **Final grade:** 100/100 cum Laude | **Level in EQF:** EQF level 4

Study Abroad Experience

Port Lincoln High School [07/2017 – 12/2017]

Address: 10 Ruskin Rd, 5606 Port Lincoln (Australia)

TRAINING AND SUMMER SCHOOLS - WITH POSTER PRESENTATIONS

[31/08/2025 – 05/09/2025]

Modern Wavefunctions Methods in Electronic Structure Theory Summer School

University of Pisa, Pisa, Italy

POSTER PRESENTATION: Savarese, A.; Melega, L.; Lipparini, F. *A preliminary implementation of the (T) correction to the CCSD energy with Cholesky-decomposed ERIs*.

[24/06/2025 – 26/06/2025]

COST COSY School CPCS 2025 "Computational Physics of Confined Systems: From Life to Material Sciences"

Online

[16/06/2025 – 18/06/2025]

COST COSY Training School “Fundamental Insights to Weak Interactions: Interplay of Theory and Spectroscopic Experiments”

Iława, Poland

CONFERENCES AND SEMINARS - WITH INVITED TALKS

[09/07/2025 – 11/07/2025]

3rd General Meeting of the "COSY" COST Action

Bologna, Italy

INVITED TALK: Savarese, A.; Alessandrini, S.; Puzzarini, C. "*Identification of the Best Candidates for Radioastronomical Detection within the C3H6O2 Isomer Family*".

[08/07/2025]

2nd WG5 Meeting – Confined Systems in Astrochemistry

Bologna, Italy

SKILLS

Informatics skills:

- Programming languages: Fortran, Python
- Markup languages: LaTex
- Code parallelization: OpenMP
- Operating systems: Linux OS
- Computer Software: Microsoft Office Suite - Word, Excel, PowerPoint, Outlook; iWork - Pages, Numbers, Keynote
- Quantum Chemistry programs: CFOUR, Gaussian, CREST, PSI4
- Chemistry software: PGOPHER, Pickett's SPFIT/SPCAT, LLWP, MestReNova, ChemSketch, ChemDraw, ChimeraX
- Bibliography Search Tools: Scifinder-*n*, Scopus, Google Scholar

Laboratory instrumentations and techniques

- Usage of millimiter-wave frequency-modulation spectrometer
- Flash-vacuum pyrolysis
- Usage of high-resolution and low-resolution SSNMR spectrometers

LANGUAGE SKILLS

Mother tongue(s): Italian

Other language(s):

English	German
LISTENING C2 **READING** C2 **WRITING** C2	**LISTENING** A1 **READING** A1 **WRITING** A1
SPOKEN PRODUCTION C2 **SPOKEN INTERACTION** C2	**SPOKEN PRODUCTION** A1 **SPOKEN INTERACTION** A1

Levels: A1 and A2: Basic user; B1 and B2: Independent user; C1 and C2: Proficient user

LANGUAGE CERTIFICATIONS

English Certifications

- Cambridge English C2 Proficiency Qualification [12-2018]
- IELTS: Overall Band Score 8.5/9 [09-11-2024]

Link: https://europa.eu/europass/eportfolio/screen/share/documents/4b0c5e12-faf5-454f-9034-455b0bb035a1?lang=en

MEMBERSHIPS

[11/2024 – Current]
Mensa Italy-High I.Q. Society

OTHER

RESEARCH INTERESTS:

- **Astrochemistry**
- Molecular spectroscopy
- Implementation of new algorithms for computational chemistry
- Atmospheric chemistry, chemistry-climate connection