

# Giacomo Botti



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## PERSONAL

Born on 06/07/1995 in Fidenza (PR)  
Italian citizen, lives in Castell'Arquato (PC)  
Speaks Italian, English, Spanish  
Classical Guitarist, Calligrapher, Baker  
Dungeon Master

## INTERESTS

Quantum dynamics  
Nuclear quantum effects  
Vibrational spectroscopy  
L<sup>A</sup>T<sub>E</sub>X & Co.  
Data visualization

## MOTIVATION

I am a Postdoctoral fellow in theoretical chemistry. I am a researcher in the field of quantum dynamics. I am always ready to learn new techniques, discover new systems to simulate and develop new solutions to unsolved problems.

## CAREER

**PostDoc**, *University of South Carolina, June 2025 –*

I am working with professor Sophya Garashchuk in developing theory and code for the quantum-trajectory adaptable Gaussian (QTAG) basis.

## EDUCATION

**Ph.D.** *in Chemistry, Università degli Studi di Milano, July 2024*

Thesis title: *Semiclassical vibrational spectroscopy of biomolecular systems*

My PhD scholarship was financed by INPS (Italian National Social System) after a competitive selection. I began my PhD by developing a software to perform an Adiabatic Switching dynamics using *ab initio* potential energy and forces. This allowed me to improve the initial conditions for the semiclassical trajectory, that are fundamental when adopting a single trajectory semiclassical method, such as Ceotto's Multiple Coherent Semiclassical Initial Value Representation (MCSCIVR).[5] While testing this code, I discovered

some discrepancies between my simulated vibrational spectra for the amino acid proline and the experimental assignment. This led to further investigations and to the complete assignment of proline vibrational spectrum using both semiclassical vibrational spectroscopy and classical dipole-dipole autocorrelation function.[4] As part of my scholarship, I moved to Perugia for six months to work with Prof. M.N. Fagnas Lago, A. Lombardi and M. Paolantoni on the preliminary stage of the construction of a dedicated force field for dimethyl sulfoxide and water mixtures, to be tested against state-of-the-art experimental spectra. In Perugia I have learned the basics of force field parametrization, along with the study of microsolvated systems using vibrational spectroscopy. Also as part of my scholarship, I spent three months at CNRS Sorbonne Université in Dr. F. Finocchi's group, investigating the presence of nuclear quantum effects in guanine-cytosine pairs IR-UV hole-burning spectra.[2] This allowed me to see how other path-integral-based methods were used for simulating nuclear quantum effects. Back in Italy, I used Adiabatic Switching to compute the vibrational eigenvalues of formaldehyde, as part of a collaboration whose goal was proving the differences between classical mechanics and quantum mechanics methods in vibrational spectroscopy.[3] I then started applying semiclassical dynamics to the rather universal resonance recently reported by Suhm *et al.* in carbonyl monohydrates. Since I am using *ab initio* semiclassical dynamics, this requires a careful selection of the initial conditions for the single trajectory so that the resonance state could be detected. In addition, I am using the theory of classical anharmonic oscillator to explain the presence of combination bands in vibrational spectra simulated with classical mechanics.

### **M.Sc.** cum laude in *Chemical Sciences, Università degli Studi di Milano, October 2019*

Thesis title: *Dipendenza delle frequenze di vibrazione dal livello di teoria elettronica: costruzione e studio semiclassico su una serie di superfici analitiche per lo stato elettronico fondamentale della formaldeide (Vibrational frequencies dependence on the level of electronic theory: construction and semiclassical study on a series of analytical surfaces for the electronic ground state of formaldehyde)*

During my M.Sc. degree under the supervision of R.Conte and M.Ceotto, I built several potential energy surfaces (PES) for formaldehyde using Bowman's Permutationally Invariant Polynomials (PIP) approach. The PES were built from the same set of geometries, but using different *ab initio* energies and numbers of polynomial terms. The PES allowed me to test semiclassical dynamics accuracy with respect to the level of theory, without resorting to a single-trajectory method. By building the PES, I was able to learn the basics of PIP fitting and how to script and automatize many tasks using BASH. Finally, I computed the semiclassical vibrational spectra of formaldehyde using the PES that I fitted.[6]

### **B.Sc.** cum laude in *Chemistry, Università degli Studi di Milano, October 2017*

Thesis title: *Un nuovo approccio per velocizzare la stima degli hessiani nella dinamica semiclassica (A new approach to speed up the Hessian matrices estimate in semiclassical dynamics)*

During my B.Sc. degree under the supervision of R.Conte and M.Ceotto, I contributed to the development of the Hessian Database protocol to speed up semiclassical dynamics using Herman-Heller-Kluk-Kay propagator. My task was to write some database store-and-fetch algorithms into a FORTRAN code and then testing them on molecular systems to find the most suitable one for our needs. This allowed me to learn both the FORTRAN language and the fundamentals of semiclassical dynamics.[7]

## PUBLICATIONS

### *Journal Articles*

1. R. Conte, G. Mandelli, **G. Botti**, D. Moscato, C. Lanzi, M. Cazzaniga, C. Aieta, and M. Ceotto, "Semi-classical description of nuclear quantum effects in solvated and condensed phase molecular systems", *Chemical Science* **16**, 20–28 (2025)

The investigation of nuclear quantum effects in solvated systems is still a challenge. In this perspective, we demonstrated the validity of semiclassical method for treating nuclear quantum effects both in vibrational spectroscopy and reaction kinetics. My contribution was using semiclassical initial value representation to reproduce the quantum vibrational features found in the spectra of carbonyl monohydrates, in particular the combination band between a libration mode and the water bending overtone. This combination band resonates with the hydrogen-bonded OH stretching, borrowing its intensity. Since this combination band involves an overtone, it cannot be properly described without quantum effects. We conclude that semiclassical approaches do account for real-time quantum contributions and are expected to point out the importance of nuclear quantum effects in complex systems for a wider range of chemical properties.

2. **G. Botti**, M. Ceotto, and R. Conte, "Investigating the Spectroscopy of the Gas Phase Guanine–Cytosine Pair: Keto versus Enol Configurations", *The Journal of Physical Chemistry Letters* **14**, 8940–8947 (2023)

A tunneling mechanism has been proposed for the double proton hopping of guanine-cytosine pair, that could facilitate base mismatch and lead to point mutations in DNA. In this paper, I used *ab initio* semiclassical vibrational spectroscopy to investigate the presence of tunneling in the IR-UV hole-burning spectra of gas-phase guanine-cytosine pair. By comparing the semiclassical spectra with both the velocity autocorrelation spectra and the experimental ones, I was able to confirm the previous experimental assignment and to exclude the presence of the tunneling product and of any other tunneling sign in the experimental spectrum.

3. R. Conte, C. Aieta, **G. Botti**, M. Cazzaniga, M. Gandolfi, C. Lanzi, G. Mandelli, D. Moscato, and M. Ceotto, "Anharmonicity and quantum nuclear effects in theoretical vibrational spectroscopy: a molecular tale of two cities", *Theoretical Chemistry Accounts* **142**, 53 (2023)

The inclusion of nuclear quantum effects is fundamental in the simulation of vibrational spectra. This paper investigates the differences between methods based on classical mechanics and methods capable of including quantum effects. My contribution was applying adiabatic switching quantization to the calculation of formaldehyde vibrational eigenvalues. The conclusions were that while the classical methods cannot reproduce nuclear quantum effects and heavily depend on the simulation energy, methods that are derived from Schrödinger equation, such as semiclassical initial value representation, include quantum effects such as zero point energy, overtones and combination bands, and their results do not depend on the temperature.

4. **G. Botti**, C. Aieta, and R. Conte, "The complex vibrational spectrum of proline explained through the adiabatically switched semiclassical initial value representation", *The Journal of Chemical Physics* **156**, 164303 (2022)

Proline is the cornerstone of proteins, playing a pivotal role in protein folding, regulation of metabolism and asymmetric catalysis. Nonetheless, its vibrational spectrum was not assigned on solid grounds and the presence of more than one conformer was still a matter of discussion. In this paper, I used the recently developed *ab initio* adiabatic switching semiclassical dynamics to obtain an accurate estimate of proline vibrational frequencies. The thorough assignment concluded that there are two conformers in the experimental spectrum, one of them characterized by an elusive OH stretching signal due to an internal hydrogen bond.

5. **G. Botti**, M. Ceotto, and R. Conte, "On-the-fly adiabatically switched semiclassical initial value representation molecular dynamics for vibrational spectroscopy of biomolecules", *The Journal of Chemical Physics* **155**, 234102 (2021)

In *ab initio* semiclassical spectroscopy, the spectrum is collected from a single, tailored trajectory using methods such as Ceotto's MCSCIVR. However, classical trajectories are inherently chaotic, so the choice of the quantized initial conditions is crucial. The use of an adiabatic switching procedure

can improve the initial conditions quantization, thus reducing the chaotic behaviour. In this paper, I implemented adiabatic switching with *ab initio* potential energies and forces and tested its capabilities on a series of molecular systems. On-the-fly adiabatic switching has proven to be a relatively cheap improvement for *ab initio* semiclassical vibrational spectroscopy and can now be applied using both NWChem and ORCA suites.

6. R. Conte, **G. Botti**, and M. Ceotto, “Sensitivity of semiclassical vibrational spectroscopy to potential energy surface accuracy: a test on formaldehyde”, *Vibrational Spectroscopy* **106**, 103015 (2020)

When running semiclassical dynamics on-the-fly, one has to compromise between the computational effort and the accuracy of the *ab initio* energy. To understand the effects of the level of theory on the semiclassical vibrational spectrum, we compared the spectra of formaldehyde, obtained with Permutationally Invariant Polynomials (PIP) PES. These PESs were fitted on around 34000 single point energies computed with different basis sets on DFT, MP2 and CCSD(T) level of theory. In this paper, I computed the single point energies and Morse coordinates required for the PIP fitting. I then used the PIP PES to compute the semiclassical vibrational spectra of formaldehyde. From this comparison, it was concluded that the main factor in semiclassical spectra accuracy is the accuracy of the potential, but – even at DFT level – semiclassical methods are a drastic improvement with respect to other more common methods, such as harmonic frequencies.

7. R. Conte, F. Gabas, **G. Botti**, Y. Zhuang, and M. Ceotto, “Semiclassical vibrational spectroscopy with Hessian databases”, *The Journal of Chemical Physics* **150**, 244118 (2019)

One of the main bottlenecks in semiclassical dynamics is the computation of the Hessian matrices at each step of the trajectory. These matrices are required to evolve the prefactor, which adds quantum effects on classical trajectories. To cut the computational time, one can recycle the computed Hessian matrices, exploiting the trajectory quasi-periodicity. This method is called Hessian Database. In this paper, I helped establishing the Hessian Database procedure by testing multiple store-and-fetch algorithms, finally selecting the best one that was then optimized and adapted for on-the-fly *ab initio* dynamics. Hessian Database is now fundamental for using *ab initio* semiclassical vibrational spectroscopy on systems of medium-to-large size.

## Posters

**G. Botti**, C. Aieta, M. Ceotto, and R. Conte, *Using ASSCIVR to understand proline vibrational spectrum*, presented at Mol Sim Eng 2023 (Politecnico di Milano – Milan, Italy), Oct. 2023

**G. Botti**, M. Ceotto, and R. Conte, *On-the-fly adiabatically switched semiclassical dynamics for vibrational spectroscopy*, presented at Capturing Anharmonic Vibrational Motion in First-Principles Simulations (Online), Dec. 2022

**G. Botti**, M. Ceotto, and R. Conte, *Using ASSCIVR to understand proline vibrational spectrum*, presented at Virtual Winter School of Computational Chemistry (Online), Feb. 2022

## Works in progress

**G. Botti**, L. Pacifici, M. Paolantoni, M. N. F. Lago, A. Lombardi, M. Ceotto, and R. Conte, “Investigation on the microsolvation of dmsol using experimental and theoretical vibrational spectroscopy”, In progress  
Dimethyl sulfoxide (DMSO) and water mixtures are highly not ideal and present a very low freezing eutectic point that makes them priceless in tissue preservation. The goal of this collaboration is to investigate DMSO microsolvation, clusterization and finally bulk solvation by combining solute-correlated IR spectroscopy, force field molecular dynamics and *ab initio* semiclassical vibrational spectroscopy.

**G. Botti**, G. Mandelli, M. Ceotto, and R. Conte, “Using semiclassical vibrational spectroscopy to unravel the rather universal Darling-Dennison resonance in carbonyl monohydrates”, In progress

Recently, a rather universal Darling-Dennison resonance in carbonyl monohydrates has been reported by Suhm and coworkers. Since this resonance involves the combination band between a water libration and the bending overtone, it is a strictly quantum feature. I aim to use *ab initio* semiclassical vibrational spectroscopy to catch this rather universal resonance, proving once again the necessity to include nuclear quantum effects in vibrational simulations. Some results were presented in Ref. [1]

**G. Botti**, M. Ceotto, and R. Conte, “Demonstrating that the so-called classical combination bands and overtones are effects of the potential anharmonicity”, In progress

When analyzing classical velocity autocorrelation spectra, one can find signals centered at the sum of the fundamental frequencies. These signals are often mistaken as quantum overtones and combinations bands. Instead, these are classical combination frequencies that appear even in the analytical solution for the anharmonic oscillator equation of motion. In this project, I want to simulate the classical velocity autocorrelation function of some analytical and molecular systems. By comparing these spectra with both semiclassical and DVR ones, I could demonstrate that the combination frequencies appearing in the classical spectra are not related to any excited vibrational quantum state.

## TEACHING EXPERIENCE

**03.2023 – 06.2023** *Teaching Assistant* at Dipartimento di Chimica, Università degli Studi di Milano (Milan, Italy). I held supplementary classes for the laboratory of Numerical Analysis (“*Calcolo Numerico*”) for the B.Sc. in Chemistry and Industrial Chemistry. I also presented some chemical applications of the course topics.

**12.2021 – 04.2022** *Test di Autovalutazione in Piano Lauree Scientifiche* at Dipartimento di Chimica, Università degli Studi di Milano (Milan, Italy). I helped building a database of questions to evaluate high school students interest for chemistry.

**09.2021 – 04.2022** *OFA Tutor* at Dipartimento di Scienze Agrarie ed Ambientali, Università degli Studi di Milano (Milan, Italy). I provided mock tests and supplementary classes to the freshmen of the agronomy B.Sc., which did not pass the mathematics section of the admission exam. I also helped in writing new questions for the online test and provided assistance during the exam.

**03.2018 – 04.2018** *Chemistry Olympics Coach* at LSS “L. Respighi” (Piacenza, Italy). I prepared a selected group of high school students for the regional-level tournament of Italian chemistry Olympics. I assisted the students in answering the Olympics quizzes, and provided classes on the advanced topics not covered in classes.

## AWARDS

**2020** *PhD Scholarship* as part of a hundred PhD scholarships for research in industry 4.0, sustainable development and welfare, awarded to sons and orphans of government employees (link to the Italian page). I won with the project “*Semiclassical spectroscopy of high dimensional molecular and supra-molecular systems*”.

**2013** *XXV edition of “I giovani e le scienze”*, with the project “*Sulle orme di Leidenfrost*” (On Leidenfrost’s footsteps); I was awarded with the participation at Expo-sciences International 2013, ACTVET UNESCO Milset, Abu Dhabi.

## COMPUTER SKILLS

***Ab initio* software** I use GAUSSIAN, NWChem and ORCA for computing *ab initio* energies, gradients, Hessians and for propagating *ab initio* Born-Oppenheimer dynamics. I visualize molecular geometries using VMD and PYMOL.

**Programming languages** I mainly write codes in FORTRAN, but I use both PYTHON and BASH for data handling and scripting. I took MATLAB classes as part of my B.Sc. and C classes as part of my M.Sc. During my PhD I took a PYTHON beginner course. I also use my PYTHON codes in some of my hobbies. I used MATLAB as *teaching assistant* for the laboratory of Numerical Analysis (“Calcolo Numerico”). I shared most of my codes to the other members of the CeottoGroup using GITLAB. I organize my work on GITHUB.

**Writing, drawing and plotting** I began using L<sup>A</sup>T<sub>E</sub>X in high school and I have never stopped since, creating multiple templates to match my needs. I recently started using MARKDOWN in Dropbox Paper for shared documents, both for work and leisure. I make my presentations with BEAMER by using my own template. I draw most of my images with TIKZ (sometimes with an help from GEOGEBRA) and plot my data with PGFPLOTS. Before I used XMGRACE and MATPLOTLIB. I still use INKSCAPE for more elaborated images.

**Communication** I got proficient in using both ZOOM and MICROSOFT TEAMS, and I use DISCORD with my friends.

**Productivity Software** I use GOOGLE DOC SHEET to organize my data. I used MICROSOFT OFFICE EXCEL as *teaching assistant* for the laboratory of Numerical Analysis (“Calcolo Numerico”). I organize my scientific library using ZOTERO.