

MARCO MENDOLICCHIO | CV

- Address: Via Consoli del Mare 2, 56123 Pisa (PI), Italy
- Born on: 12/10/1992
- E-mail: marco.mendolicchio@sns.it
- Research field: Theoretical and computational chemistry



EDUCATION AND TRAINING

- 2016 - Present **PhD position**, Scuola Normale Superiore, Pisa (Italy)
 - Course: Methods and Models for Molecular Sciences
 - PhD advisor: Prof. Vincenzo Barone
- 2011 - 2016 **Diploma di licenza**, Scuola Normale Superiore, Pisa (Italy)
 - Final exam of the undergraduate program of Scuola Normale Superiore
- 2014 - 2016 **Master's degree in Chemical Sciences (Physical Chemistry)**, University of Pisa (Italy)
 - Final grade: 110/110 *cum laude*
 - Advisor: Prof. Vincenzo Barone
 - Thesis: Anharmonicity effects on the structural and vibrational properties of molecular systems in different electronic states
- 2011 - 2014 **Bachelor's degree in Chemical Sciences**, University of Pisa (Italy)
 - Final grade: 110/110 *cum laude*
 - Advisor: Prof. Vincenzo Barone
 - Thesis: General fitting approach for anharmonic force fields
- 2006 - 2011 **High-school degree**, Liceo scientifico tecnologico Enrico Fermi, Lucca (Italy)
 - Final grade: 86/100

RESEARCH ACTIVITY

My research activity focuses on the development of computational methods for the inclusion of anharmonicity effects on the calculation of structural and vibrational properties of polyatomic molecular systems. During my bachelor and master degrees projects, I worked on different strategies for computing anharmonic force fields by fitting and numerical differentiation approaches, aimed at the calculation of accurate vibrational spectra. In addition, during my master degree project I developed a new software called Molecular Structure Refinement (MSR) for the calculation of accurate equilibrium molecular structures by means of the so-called semi-experimental approach. In this context, the attention has been mainly focused on the development of efficient strategies for the set of internal coordinates to be employed in the refinement procedure, by making proper use of molecular symmetry. In the second place, a complete support of hybrid strategies for treating large and flexible systems have been studied and included as well. The MSR software is being used in our group to build a database of accurate molecular geometries, which is of fundamental relevance to benchmark new computational protocols as well as to test the reliability of approximate models for larger systems. Currently, I am working on new computational strategies to treat medium-sized molecular systems presenting some flexibility, and thus are unsatisfactorily described at the vibrational second-order perturbation theory (VPT2) level.

»»» PUBLICATIONS ON INTERNATIONAL PEER-REVIEWED JOURNALS

- 2015 ▶ A. Baiardi, M. Mendolicchio, V. Barone, G. Fronzoni, G.A. Cardenas Jimenez, M. Stener, C. Grazioli, M. de Simone, M. Coreno, **Vibrationally resolved NEXAFS at C and N K-edges of pyridine, 2-fluoropyridine and 2,6-difluoropyridine: A combined experimental and theoretical assessment**, *The Journal of Chemical Physics*, 103, 204102 (2015)
- 2016 ▶ F.A. Gianturco, M. Satta, M. Mendolicchio, F. Palazzetti, A. Piserchia, V. Barone, R. Wester, **Exploring a chemical route for the formation of stable anions of polyynes [C_nH⁻ (n = 2, 4)]**, *The Astrophysical Journal*, 830, 2 (2016)
- ▶ E. Penocchio, M. Mendolicchio, N. Tassinato, V. Barone, **Structural features of the carbon-sulfur chemical bond: A semi-experimental perspective**, *Canadian Journal of Chemistry*, 94, 1065 (2016)
- 2017 ▶ M. Mendolicchio, E. Penocchio, D. Licari, N. Tassinato, V. Barone, **Development and implementation of advanced fitting methods for the calculation of accurate molecular structures**, *The Journal of Chemical Theory and Computation*, 13, 3060 (2017)
- 2018 ▶ A. Melli, M. Melosso, N. Tassinato, G. Bosi, L. Spada, J. Bloino, M. Mendolicchio, L. Dore, V. Barone, C. Puzzarini, **Rotational and Infrared Spectroscopy of Ethanimine: A Route toward Its Astrophysical and Planetary Detection**, *The Astrophysical Journal*, 855, 123 (2018)

»»» PARTICIPATION AT NATIONAL CONFERENCES

- 2015 ▶ **Winter Modeling 2015 – Complex Molecular Systems: Accuracy and Interpretation**, Scuola Normale Superiore, Pisa (Italy), December 18, 2015
- 2017 ▶ **Y-Rich Workshop** of the Italian Chemical Society, Roma (Italy), June 23, 2017
- ▶ **Dalla modellizzazione computazionale alla realtà virtuale attraverso spettroscopia astrochimica**, Napoli (Italy), November 7–9, 2017

»»» PRESENTATIONS IN NATIONAL AND INTERNATIONAL CONFERENCES

- 2015 ▶ M. Mendolicchio, A. Baiardi, J. Bloino "A fitting approach for anharmonic force fields", 3rd National Meeting of the Theoretical and Computational Chemistry division of the Italian Chemical Society, Roma (Italy), December 14–16, 2015 · **Poster**
- 2017 ▶ M. Mendolicchio, N. Tassinato, V. Barone "MSR: a new software for the calculation of accurate molecular structures", *Workshop DREAMS@Anacapri*, Isle of Capri (Italy), April 20–22, 2017 · **Poster**
- ▶ A. Balbi, N. Tassinato, M. Mendolicchio, C. Puzzarini, V. Barone "Accurate quantum-chemical spectroscopic characterization of interstellar methanimidic acid", *25th Colloquium on High-Resolution Molecular Spectroscopy*, Helsinki (Finland), August 20 - 25, 2017 · **Poster**
- ▶ M. Mendolicchio, N. Tassinato, V. Barone "Development and implementation of new computational methods for the calculation of accurate equilibrium molecular structures", *25th Colloquium on High-Resolution Molecular Spectroscopy*, Helsinki (Finland), August 20 - 25, 2017 · **Poster**
- ▶ M. Mendolicchio, R. Bousseffi, N. Tassinato, V. Barone "New computational tools for the determination of molecular structures: the MSR software", ERC AdG – Barone – DREAMS: final meeting, *Advances in computational modelling: from isolated molecules to soft matter*, Pisa (Italy), November 20 - December 2, 2017 · **Poster**
- 2018 ▶ M. Mendolicchio, N. Tassinato, V. Barone "Determination of accurate structural parameters through the semi-experimental approach: application to astrochemical molecules", *ASTRO-Winter Modeling Advances in computational & experimental modeling: Application to Astrochemistry*, Bologna (Italy), February 14–16, 2018 · **Talk**

»»» INVITED

- 2017 » M. Mendolicchio, N. Tasinato, V. Barone "New models and computational strategies for molecular structure prediction", XXVI National Conference of the Italian Chemical Society, Paestum (Italy), September 10–14, 2017 · **Talk**

»»» HONORS AND AWARDS

- 2017 » **Pier Luigi Nordio Award** prize awarded by Theoretical and Computational Chemistry Division of the Italian Chemical Society (SCI) for the best Master's degree thesis in theoretical and computational chemistry

»»» TEACHING ACTIVITY

- 2017 **Theoretical models for the simulation of vibrational spectra (8h)**, University of Pisa (Italy)
 » Series of didactic seminars
- 101° Corso di orientamento universitario (training course for high-school students applying to the Scuola Normale Superiore)**, San Miniato (Italy), 26 June – 1 July, 2017
 » Tutor: introductory lessons for high-school students on theoretical chemistry
 » Didactic seminar – topic: "Spectroscopy: a tool to probe the matter"
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- 2018 **Computational spectroscopy (8h)**
 » Series of lectures within the course "Computational spectroscopy", Scuola Normale Superiore, Pisa (Italy)

»»» THESIS SUPERVISION

- 2017 **Master of Science thesis**, Scuola Normale Superiore, Pisa (Italy)
 » Candidate: Alice Balbi
 » Topic: Quantum-chemical protocols for structural and ro-vibrational properties of small to medium sized molecules of bio- and astro-chemical relevance

»»» INSTITUTIONAL ROLES

- 2014 - 2015 **Member of the class council**, Scuola Normale Superiore, Pisa (Italy)
 » Role: students' delegate
- 2015 - 2016 **Member of the academic senate**, Scuola Normale Superiore, Pisa (Italy)
 » Role: students' delegate
- 2017 - Present **Member of the funding committee**, Scuola Normale Superiore, Pisa (Italy)

»»» COMPUTATIONAL SKILLS

- Programming languages » Good skills in Visual Basic
 » Advanced skills in Fortran 77/90/95 and Python
 » Shell scripting
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- Operating systems » Good skills in GNU/Linux, and MS Windows
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- Digital skills » Advanced knowledge of common text editors (Office, Latex, Beamer)
 » Graphics (Inkscape, Gimp, Scribus)

»»» LANGUAGES

- Italian Mother tongue
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- English Good skills in reading, writing and oral expression