Marco MENDOLICCHIO

PhD in Methods and Models for Molecular Sciences

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Born on October 12, 1992 in Lucca (Italy) marco.mendolicchio@sns.it
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Research activity

Marco Mendolicchio's research activity largely focuses on astrochemistry, where reaction kinetics and spectroscopy are important for characterizing reaction mechanisms as well as individuating molecules and possible reaction intermediates in the interstellar medium (ISM) or planetary atmospheres. In this kind of research, microwave and infrared spectroscopies play a crucial role in driving the interpretation of observational spectra. However, the latter are the result of an unknown mixture of species, in conditions which may be difficult to reproduce in the laboratory. He is working on the development of reliable computational models able to provide accurate predictions of the transition energies and intensities, required to drive experiments and assist the interpretation of the spectrum. Concerning rotational spectroscopy, he is currently developing and implementing the MSR (Molecular Structure Refinement) software for the calculation of accurate structural parameters of medium-to-large sized molecular systems. The MSR software is being used in our group to build a database of accurate molecular geometries, which can be used in several applications such as the benchmark of new computational protocols as well as to test the reliability of approximate models. In addition, he is working on the development and application of accurate methods for the simulation of vibrational spectra and the analysis of reaction kinetics:

- development of algorithms for the calculation of anharmonic force fields of any order for both perturbative and variational calculations;
- development of computational methods for the calculation of anharmonic infrared spectra of symmetric top molecules at the vibrational second-order perturbation theory (VPT2) level;
- development and implementation of computational methods (perturbative and variational) for the calculation of accurate anharmonic infrared spectra of small-to-medium sized molecular systems presenting some flexibility, which are unsatisfactory described purely at the VPT2 level;

Finally, he is working on the definition of computational protocols for the simulation of electronic high-energy spectra, including X-ray absorption near edge structure (NEXAFS), X-ray photoelectron spectroscopy (XPS) and X-ray Absorption Spectroscopy (XAS).

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)**
- Degree certificate for attending the undergraduate course at Scuola Normale Superiore

2014 – 2016 | **Master's degree in Chemical Sciences (Physical Chemistry), University of Pisa, 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, 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

Participation to National and International Schools

2019 | Molecular Response Properties Winter School (MRPWS 2019), Bardufoss (Norway), January 14 – 18, 2019
- Lectures and tutorial lessons

2018 | Summer School: Modern Wavefunctions Methods in Electronic Structure Theory (MWM 2018), Wissenschaftspark Gelsenkirchen (Germany), September 30 – October 5, 2018
- Lectures and tutorial lessons
- Poster presentation

Publications in International Peer-Reviewed Journals

2019
- M. Mendolicchio, A. Baiardi, G. Fronzoni, M. Stener, C. Grazioli, M. de Simone, V. Barone, **Theory meets experiment for unravelling the C1s X-ray Photoelectron Spectra of pyridine, 2-fluoropyridine and 2,6-difluoropyridine**, *The Journal of Chemical Physics*, 151, 124105 (2019)

2018
- D. A. Obenchain, L. Spada, S. Alessandrini, S. Rampino, S. Herbers, N. Tasinato, M. Mendolicchio, P. Kraus. J. Gauss, C. Puzzarini, J. Grabow, V. Barone, **Unveiling the Sulfur-Sulfur Bridge: Accurate Structural and Energetic Characterization of a Homochalcogen Intermolecular Bond**, *Angewandte Chemie*, 57, 15822 (2018)
- D. Licari, M. Fusè, A. Salvadori, M. Mendolicchio, N. Tasinato, G. Mancini, V. Barone, **Towards the SMART workflow system for computational spectroscopy**, *Physical Chemistry Chemical Physics*, 20, 26034 (2018)
- A. Melli, M. Melosso, N. Tasinato, 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)

2017
- M. Mendolicchio, E. Penocchio, D. Licari, N. Tasinato, 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)

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_n H - (n = 2, 4)]**, *The Astrophysical Journal*, 830, 2 (2016)
- E. Penocchio, M. Mendolicchio, N. Tasinato, V. Barone, **Structural features of the carbon-sulfur chemical bond: A semi-experimental perspective**, *Canadian Journal of Chemistry*, 94, 1065 (2016)

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)

Participation to National and International Conferences

2017
- **Y-Rich Workshop** of the Italian Chemical Society, Roma (Italy), June 23, 2017
- **Dalla modellizzazione computazionale alla realtà virtuale attraverso spettroscopia astrochimica**, Naples (Italy), November 7 – 9, 2017

2015
- **Winter Modeling 2015 – Complex Molecular Systems: Accuracy and Interpretation**, Scuola Normale Superiore, Pisa (Italy), December 18, 2015

Presentations in National and International Conferences

2019
- M. Mendolicchio, J. Bloino, V. Barone **Building a reliable theoretical companion for astrochemical investigations**, 6th National Meeting of the Theoretical and Computational Chemistry division of the Italian Chemical Society, Rende (Italy) September 19 – 20, 2019 · **Oral presentation**

- M. Mendolicchio, J. Bloino, V. Barone **New Tools for Computational Astrochemistry: the VMS-Astro Project**, 12th European Conference on Computational and Theoretical Chemistry (EUCO-CTC), Perugia (Italy) September 1 – 5, 2019 · **Oral presentation**

- M. Mendolicchio, J. Bloino, V. Barone **Anharmonic vibrational treatment of linear, symmetric and asymmetric molecules**, Young Researchers Meet Spectroscopy – YRMS@2019, Pisa (Italy) April 4 – 5, 2019 · **Oral presentation**

- M. Mendolicchio, J. Bloino, V. Barone **Toward the unified model for the anharmonic spectra of linear, symmetric and asymmetric molecules**, Winter Modeling 2019, Napoli (Italy), February 14, 2019 · **Oral presentation**

2018

- M. Mendolicchio, J. Bloino, V. Barone **New Computational Strategies for the Calculation of Anharmonic Force Fields**, 5th National Meeting of the Theoretical and Computational Chemistry division of the Italian Chemical Society, Trieste (Italy), September 19 – 21, 2018 · **Oral presentation**

- M. Mendolicchio, N. Tasinato, V. Barone **The MSR Route to Accurate Equilibrium Molecular Structures Through the Semi-Experimental Approach**, XXXIV European Congress on Molecular Spectroscopy (EUCMOS) 2018, Coimbra (Portugal), August 19 – 24, 2018 · **Oral presentation**

- M. Mendolicchio, N. Tasinato, V. Barone **Computational strategies for the calculation of accurate equilibrium molecular structures**, Theoretical Chemistry and Computational Modelling Final Workshop ITN-EJD, Pisa (Italy), July 23 – 25, 2018 · **Oral presentation (Invited PhD student)**

- M. Mendolicchio, J. Bloino, N. Tasinato, V. Barone **Anharmonicity Effects on the Structural and Vibrational Properties of Molecular Systems of Astrochemical Interest**, Astrochem2@2018 – II Italian Workshop on Astrochemistry "Chemical Evolution in our Galaxy: Spectroscopy, Observations and Reactivity", Follonica (Italy), June 13 – 16, 2018 · **Oral presentation**

- M. Mendolicchio, N. Tasinato, 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 · **Oral presentation**

2017

- M. Mendolicchio, R. Boussessi, N. Tasinato, 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 presentation**

- M. Mendolicchio, N. Tasinato, 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 presentation**

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 presentation**

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 · **Oral presentation**

Honors and Awards

2018

- **Finalist of the first edition of the contest ChiMiCapisce** organized by the Young Group of the Italian Chemical Society for divulgation skills of chemical sciences

2017

- **Pier Luigi Nordio Award** prize awarded by the Theoretical and Computational Chemistry Division of the Italian Chemical Society for the best Master's degree thesis in theoretical and computational chemistry of the academic year 2016/2017

Teaching Activity

2019

106° Corso di orientamento universitario (training course for high-school students applying to the Scuola Normale Superiore), San Miniato (Italy), June 25 – 30, 2019
- Tutor: introductory lessons for high-school students on theoretical chemistry

Computational Spectroscopy (13h), Scuola Normale Superiore, Pisa (Italy)
- Series of lectures (academic year: 2018/2019)

Scientific programming (16h), Scuola Normale Superiore, Pisa (Italy)
- Co-supervision in a series of practical sessions of exercises (academic year: 2018/2019)

2018

Computational Spectroscopy (9h), Scuola Normale Superiore, Pisa (Italy)
- Series of lectures (academic year: 2017/2018)

103° Corso di orientamento universitario (training course for high-school students applying to the Scuola Normale Superiore), Follonica (Italy), June 18 – 23, 2018
- Tutor: introductory lessons for high-school students on theoretical chemistry

2017

Theoretical models for the simulation of vibrational spectra (8h), University of Pisa, Pisa (Italy)
- Series of didactic seminars (academic year: 2016/2017)

101° Corso di orientamento universitario (training course for high-school students applying to the Scuola Normale Superiore), San Miniato (Italy), June 26 – July 1, 2017
- Tutor: introductory lessons for high-school students on theoretical chemistry

Thesis Supervision

2017

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

Academic Roles

2017 – Present

Member of the funding commettee, Scuola Normale Superiore, Pisa (Italy)
- Role: PhD student's delegate

2015 – 2016

Member of the academic senate, Scuola Normale Superiore, Pisa (Italy)
- Role: Student's delegate

2014 – 2015

Member of the class council, Scuola Normale Superiore, Pisa (Italy)
- Role: Student's delegate

Computational skills

Programming
- Good skills in Visual Basic
- Advanced skills in Fortran 77/90/95 and Python 2/3

Operating systems
- Good skills in GNU/Linux and MS/Windows

Digital skills
- Advanced knowledge of common text editors (Office, Latex, Beamer)
- Graphics: Inkscape, Gimp, Scribus

Languages

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