Michele Ceotto

Curriculum Vitae

PERSONAL DATA

Place and date of birth	Conegliano, 2nd of March, 1972
Citizenship	Italian
Email address	**michele.ceotto@unimi.it**,
website	https://sites.unimi.it/ceotto/

POSITION

since 2015	ERC Consolidator Group Leader for the project SEMICOMPLEX at the Department of Chemistry, Università degli Studi di Milano (Italy)
since 2015	Associate Professor, Department of Chemistry, Università degli Studi di Milano (Italy) ("*chiamata diretta per chiara fama a Professore Associato Confermato*")
2006-2015	Assistant Professor, Department of Chemistry, Università degli Studi di Milano (Italy)

EDUCATION

2005-2006	Postdoctoral Fellow, "Center for Biophysical Modeling and Simulation", Prof. G.A. Voth's group, Dept. of Chemistry, University of Utah, Salt Lake City (USA)
2005	PhD in Chemistry, University of California at Berkeley (USA); advisor Prof. W. H. Miller, thesis's title: "Semiclassical and Quantum Instanton approximations for thermal rate constants of chemical reactions"
2000	Laurea (M.S.) in Physics (110/110), Università degli Studi di Roma "La Sapienza" (Italy)
1999	Laurea (M.S.) in Chemistry (110/110 cum laude), advisor Prof. F.A. Gianturco, Università degli Studi di Roma "La Sapienza" (Italy)
1991	Diploma, Liceo Scientifico "Guglielmo Marconi", Conegliano (Treviso, Italy)

FELLOWSHIPS AND AWARDS

2018	Abilitazione Nazionale di Professore Ordinario in Chimica, SSD CHIM/02
2018	Abilitazione Nazionale di Professore Ordinario in Fisica, SSD FIS/02
2018	Seal of excellence: Marie Skłodowska-Curie actions call H2020-MSCA-IF-2016 (as Hosting PI); Certificate delivered by the European Commission.
2017	FARE (Framework for attracting and strengthening of research excellence in Italy) – MIUR
2017	Seal of excellence: Marie Skłodowska-Curie actions call H2020-MSCA-IF-2017 (as Hosting PI); Certificate delivered by the European Commission.
2015	European Research Council (ERC): ERC Consolidator Grant 2014
2000-2005	University of California at Berkeley (USA): International student fellowship for graduate studies in Theoretical & Computational Physical Chemistry
2000	Fellowship by the "Consiglio Nazionale delle Ricerche" (CNR) for studies outside Italy
2000	European Union Training and Mobility for Researchers (TMR) Fellowship at the Consejo Superior de las Investigaciones Cientificas (CSIC) and "Istituto de Matematicas y Fisica Fundamental" (IMAFF), Prof.s Garcia-Vela and Delgado-Barrio, Madrid (Spain)
1998	Visiting student Fellowship at Department of Chemistry, University of Warwick (UK)
1992-1999	Tax-free application at the University of Rome "La Sapienza" for outstanding GPA at each academic year
1992-1999	Italian National Federation "Cavalieri del Lavoro" Fellowship: about 20 grants each year nationwide (over the entire Italian University student population). The grant includes full board, lodging, and additional academic courses during all undergraduate studies

GRANTS

2018-2020	FARE – Italian MIUR Grant, 182 340 € for the project QURE, "*A theoretical-computational study of photocatalytic remediation of polluted atmospheres*", Principal Investigator (PI)

2016-2017 LISA, Regione Lombardia, 37 200 € (1 116 668 CPU hrs), for the project GREENTI, "*Quantum mechanical investigation of active TiO_2*", PI

2015-2020 ERC Consolidator Grant 2014, 1 899 973 € for the project SEMICOMPLEX, "*Divide and Conquer ab initio Semiclassical Molecular Dynamics for Spectroscopic Calculations of Complex Systems*", Principal Investigator (PI)

2014-2015 LISA, Regione Lombardia, 63 000 € (1 800 000 CPU hrs), for the project SURGREEN, "*Quantum mechanical investigation of active TiO_2*", PI

2014-2015 SMART MAT Lab, Department of Chemistry, CARIPLO foundation, Università degli Studi di Milano, Regione Lombardia, 970 740 €, "*An Interdisciplinary Laboratory for smart materials synthesis*", Participant

2014 LISA, Regione Lombardia, 3 300 € (100 000 CPU hrs), production grant, "*Parallelization of the MultiWell Program Suite for Semiclassical Thermal Rate Constant Calculations*", PI

2014 Department of Chemistry, Università degli Studi di Milano, 6 800 €, "*Ab initio semiclassical Molecular Dynamics*", PI

2013-2014 CINECA (Italian Supercomputing Center), Università degli Studi di Milano, 9000€ (300 000 CPU hrs), "*Titania film nanotexturing for outdoor cultural heritage preservation*", PI

2013-2014 LISA, Regione Lombardia, 20 000 € (600 000 CPU hrs), for the project MATGREEN, "N*ew titania materials for environmental remediation*", PI

2011 NVIDIA, 8 000 € (Hardware), "*GPU accelerated semiclassical moelcular dynamics*", co-PI

2010 Department of Physics, Università degli Studi di Milano, 61 000 € (Ph.D. Fellowship), co-PI

2009-2013 "Cinque per Mille", Università degli Studi di Milano, 40 000 €, "*Monitoring and environmental remediation of organic and inorganic pollutants from waste waters: a theoretical and experimental approach*", co-PI

2009-2011 Ministero dell'Istruzione, dell'Università e della Ricerca (MIUR), PRIN, 117 000 €, "*DFT calculations of confined nano-systems*", Participant

2009-2014 PUR, Università degli Studi di Milano, 22 000 €, "*Nano and Micro structured multifunctional materials for energy storage and conversion and environmental remediation*", Participant

2007-2009 MIUR (PRIN), 121 000 €, "*Quantum-mechanical calculations for gas phase molecular spectra*", Participant

MAJOR COLLABORATIONS

- D. Marx (Bochum University, Germany): IR spectra calculations of biomolecules
- A. Aspuru-Guzik (Harvard University, USA): ab initio calculations for semiclassical dynamics
- W.L. Hase and Y. Zhuang (Texas Tech University, USA): hessian integrators for semiclassical molecular dynamics
- F. Grossman (Technische Universitat Dresden, Germany): hybrid semiclassical propagators
- D. Tamascelli (Università degli Studi di Milano, Italy): GPU accelerated semiclassical molecular dynamics
- L. Lo Presti (Università degli Studi di Milano, Italy): plane wave (VASP, QE) and atom-centered (CRYSTAL) DFT calculations of doped TiO_2
- S. Ardizzone and L. Falciola (Università degli Studi di Milano, Italy): characterization and photocatalysis of doped titania for photocatalytic enviromental remediation
- G. Cappelletti and P. Fermo (Università degli Studi di Milano, Italy): characterization of nano-texured titania films for outdoor cultural heritage protection
- J. Schrier (Haverford College, USA): helium isotope enrichment by resonant tunneling through nanoporous graphene bilayers
- M. Benaglia (Università degli Studi di Milano, Italy): beyond the Curtin-Hammett principle

SUPERVISION OF STUDENTS AND POSTDOCTORAL FELLOWS

Present: R. Conte (Postdoctoral Fellow), M. Micciarelli (Postdoctoral Fellow), C. D. Aieta (Postoctoral Fellow), J. Suarez (Postdoctoral Fellow), G. Bertaina (Postdoctoral Fellow), M. Cazzaniga (Postdoctoral Fellow), F. Gabas (Postdoctoral Fellow), A. Rognoni (Ph.D. student), G. Botti (Master); G. Mandelli

(Master).
Past:

2017-2018 M. Buchholz	Postdoctoral Fellow
2015-2018 G. Di Liberto	Ph.D. in Chemistry
2015-2018 F. Gabas	Ph.D. in Chemistry
2018 G. Buccella	Master Thesis in Chemistry
2018 E. Fallacara	Master Thesis in Chemistry
2018 A. Fasan	Bachelor Thesis in Chemistry
2017-2016 Huaqing Li	Postdoctoral Fellow
2107-2016 A. N. Mahmoud	Postdoctoral Fellow
2017 S. Americo	Bachelor in Chemistry
2017 G. Botti	Bachelor Thesis in Chemistry (now Master student in my group)
2016 G. Ruffa	Bachelor Thesis in Physics
2016 F. Moriggi	Bachelor and Master Thesis in Chemistry
2016 D. Balestra	Bachelor Thesis in Chemistry
2016 L. Parma	Bachelor and Master Thesis in Chemistry
2016 A. Rognoni	Bachelor and Master Thesis in Chemistry (now Ph.D. student in my group)
2016 R. Bellani	Master thesis in Chemistry
2015 G. Bruno	Bachelor Thesis in Chemistry
2015 G. Di Liberto	Bachelor and Master Thesis in Chemistry
2013 S. Mandrà	PhD Thesis in Physics (postdoctoral fellow at Harvard University, USA)
2013 F. S. Dambrosio	Bachelor Thesis in Chemistry (Ph.D at Oxford)
2010 D. Lotti	Bachelor and Master Thesis in Chemistry (PhD student at Univ. of Zurich, CH)
2010 M. Azzola	Bachelor and Master Thesis in Chemistry (Physics student)
2010 C. Aieta	Bachelor, Master Thesis and PhD in Chemistry (now postdoct in my group)
2008 S. Valleau	Bachelor and Master Thesis in Chemistry (PhD student at Harvard Univ., USA)
2007 D. dell'Angelo	Master Thesis in Chemistry (postdoctoral fellow at Univ. South Carolina, USA)

TEACHING ACTIVITIES

Università degli Studi di Milano, Italy

Since 2011	Spectroscopy (Part I): Fundamental Theory for Spectroscopic Techniques	(und. div.)
Since 2016	Lab. of Physical Chemistry A: Software for ab initio Calculations	(master div.)
Since 2015	Quantum Chemistry: ab initio methods	(master div.)
Since 2007	Theoretical Chemistry: Classical and Quantum Molecular Dynamics	(master div.)
2006-2016	Lab. Physical Chemistry I: Statistical Theory of Experimental Data Treatment	(und. Div.)
2009-10	Principles of Physical Chemistry: Atoms and Molecule	(undergraduate div.)
2011	Scuola di Dottorato in Scienze e Tecnologie Chimica, Corso di dottorato in Scienze Chimiche, “Chemistry at Surfaces: Experiments and Theory”	(PhD div.)
2013	PhD Course in Chemical Sciences, “Taking a glance on ultrasmall and ultrafast worlds: time-resolved and free-electron laser probes for chemical applications”	(PhD div.)
2015	PhD Courses in Chemical Sciences, “Physical Chemistry of Nanosized Titania: first principles calculations versus experiments”	(PhD div.)

University of California at Berkeley, USA

Fall 2004-05	Physical Chemistry Laboratory: Statistics and Thermodynamics	(undergrad. div.)
Fall 2002	Biophysical Chemistry: Principles of Thermodynamics	(upper division)
Fall 2001	Quantum Mechanics: Principles of Quantum Mechanics	**(**graduate division)
Fall 2000	Principles of Chemistry	(undergraduate division)

ORGANIZATION OF SCIENTIFIC MEETINGS

- 6-10 June 2016: CECAM Workshop: ”*Different routes to quantum molecular dynamics*”, Lausanne, Switzerland; https://www.cecam.org/workshop-1319.html
- 8 April 2016: NOBEL LECTURE Prof. Martin Karplus (Harvard University) 2013 Nobel Prize in Chemistry
- 17-21 June 2013: CECAM Workshop: ”*Many-dimensional quantum dynamics with (non)classical*

trajectories", Lausanne, Switzerland; http://www.cecam.org/workshop-0-884.html

EU-MIRATED RESPONSABILITIES

2012-present Member of the European Grid Infrastructure (EGI, www.egi.eu) CompChem (**FP7** funds)
2012-present EChem Test (a pan-European Chemistry Test): local organizer and contact point

INSTITUTIONAL RESPONSABILITIES

2016 Ph.D Committee member, Université Pierre et Marie Curie, Institut de Nanoscience de Paris
2015 Ph.D. degree Committee member, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH
2014 Master degree Committee member, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH
2012-2017 Teaching Committee of Chemistry and Industrial Chemistry (Commissione Didattica)
2012-present Committee for High Schools Orientation (Commissione Orientamento)
2012-2017 Committee for internal evaluation and planning (Comm. Valutazione e Programmazione)
2012-present "Collegio" of Doctoral School of Chemistry
2010-present Committee of Doctoral School of Chemical Science (Commissione Dottorato)
2010 Master degree Committee member, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH

EXTERNAL EXAMINER

2016 Y. Bronstein, Ph.D. exam, for the Department of Physics at UPMC (Paris, FR)
2015 M. Wehrle, Ph.D. exam, for the Department of Chemistry at EPFL (Lausanne, CH)
2014 J. Rohrbach, Master exam, for the Department of Chemistry at EPFL (Lausanne, CH)
2010 M. Wehrle, Master exam, for the Department of Chemistry at EPFL (Lausanne, CH)

EDITORIAL BOARD

Since 2013 Frontiers in Chemistry
2012-2017 Dataset Papers in Atomic and Molecular Physics

REFEREE FOR:

Institutions: Ministero dell' Istruzione, dell' Università e della Ricerca: "Futuro in Ricerca" (FIRB); "Scientific Independence of young Researchers" (SIR); PRIN; VQR; ETH Grant Research Proposal; Fondecyt Science Council - Conycyt (Chile), CECAM.
Journals: J. Chem. Phys.; J. Chem. Theory and Compu.; J. Phys. Chem.; J. Phys. Chem. Lett.; ACS Nano, J. of Material Chemistry; Mol. Phys.; International Journal of Quantum Chemistry; Chemical Sciences; RCS Adv.; Dalton Transactions; Phys. Chem. Chem. Phys.; Chemistry of Materials, Curr. Appl. Phys., Res. Chem. Intermed.
2018 **22** papers referred; 2017 **33** papers referred; 2016 **33** papers referred; 2015 **22** papers refereed; 2014 **24** papers refereed; 2013 **15** papers refereed; 2012 **5** papers referred.

MEMBERSHIP OF SCIENTIFIC SOCIETIES

2006-Present Italian Chemical Society
2002-Present American Chemical Society

PUBLICATIONS

1. F. Gabas, G. Di Liberto, and **M. Ceotto***, "Protonated glycine supramolecular systems: the need for quantum dynamics", *Journal of Chemical Physics* **150**, 224107 (2019);
2. M. Micciarelli*, F. Gabas, R. Conte, and **M. Ceotto***, "An effective semiclassical approach to IR spectroscopy", *Journal of Chemical Physics* **150**, 184113 (2019);
3. C. Aieta, F. Gabas, **M. Ceotto***, "AParallel Implementation of Semiclassical Transition State Theory", *J. Chemical Theory and Computation* **15**, 2142-2153 (2019);
4. M. Buchholz, E. Fallacara, F. Gottwald, M. Ceotto, F. Grossmann, and S. D. Ivanov, "Herman-Kluk propagator is free from zero-point energy leakage", *Chemical Physics* **515**, 231-235 (2018);

5. X. Ma, G. Di Liberto, R. Conte, W. L. Hase*, and **M. Ceotto***, "A quantum mechanical insight into S_N2 reactions: Semiclassical initial value representation calculations of vibrational features of the Cl^- … CH_3Cl pre-reaction complex with the VENUS suite of codes", *Journal of Chemical Physics* **149**, 164113 (2018);
6. F. Gabas, G. Di Liberto, R. Conte*, and **M. Ceotto***, "Protonated glycine supramolecular systems: the need for quantum dynamics", *Chemical Science* **9** (41), 7885-8026 (2018); This article is part of the themed collections: 2018 ChemSci Pick of the Week Collection, 2018 Chemical Science HOT Article Collection and journal cover;
7. M. Micciarelli*, R. Conte, J. Suarez, and **M. Ceotto***, "Anharmonic vibrational eigenfunctions and infrared spectra from semiclassical molecular dynamics", *Journal of Chemical Physics* **149**, 064115 (2018);
8. M. Buchholz, F. Grossmann, and **M. Ceotto***, "Simplified approach to the mixed time-averaging semiclassical initial value representation for the calculation of dense vibrational spectra", *Journal of Chemical Physics* **148**, 114107 (2018);
9. G. Di Liberto, R. Conte, and **M. Ceotto***, "Divide and conquer" semiclassical molecular dynamics: An application to water clusters", *Journal of Chemical Physics* **148**, 104302 (2018);
10. G. Di Liberto, R. Conte, and **M. Ceotto***, ""Divide and conquer" semiclassical molecular dynamics: A practical method for spectroscopic calculations of high dimensional molecular systems", *Journal of Chemical Physics* **148**, 014307 (2018);
11. M. Buchholz, F. Grossmann, and **M. Ceotto***, "Application of the mixed time-averaging semiclassical initial value representation method to complex molecular spectra", *Journal of Chemical Physics* **147**, 164110 (2017);
12. G. Di Liberto, V. Pifferi, L. Lo Presti*, **M. Ceotto***, and L. Falciola*, "Atomistic Explanation for Interlayer Charge Transfer in Metal–Semiconductor Nanocomposites: The Case of Silver and Anatase", *Journal of Physical Chemistry Letters* **8**, 5372-5377 (2017);
13. **M. Ceotto***, G. Di Liberto, and R. Conte, "Semiclassical "Divide-and-Conquer" Method for Spectroscopic Calculations of High Dimensional Molecular Systems", *Phys. Rev. Lett.* **119**, 010401 (2017);
14. F. Gabas, R. Conte, and **M. Ceotto***, "On-the-fly ab initio Semiclassical Calculation of Glycine Vibrational Spectrum", *J. Chem. Theory Comput.* **13**, 2378-2388 (2017);
15. C. Aieta, **M. Ceotto***, "A quantum method for thermal rate constant calculations from stationary phase approximation of the thermal flux-flux correlation function integral", *J. Chem. Phys.* **146**, 214115 (2017);
16. D. Meroni*, L. Lo Presti*, G. Di Liberto, **M. Ceotto***, R. G. Acres, K. C. Prince, R. Bellani, G. Soliveri, and S. Ardizzone, "A Close Look at the Structure of the TiO_2-APTES Interface in Hybrid Nanomaterials and Its Degradation Pathway: An Experimental and Theoretical Study", *J. Phys. Chem C*, **121**, 430-440 (2017);
17. JR Barker, TL Nguyen, JF Stanton, C Aieta, M Ceotto, F Gabas, TJD Kumar, CGL Li, LL Lohr, A Maranzana, NF Ortiz, JM Preses, JM Simmie, JA Sonk, PJ Stimac, MultiWell-2017 Software Suite, Ann Arbor, Michigan (2017)
18. G. Di Liberto, **M. Ceotto***, "The importance of the pre-exponential factor in semiclassical molecular dynamics", *J. Chem. Phys.* **145**, 144107 (2016);
19. C. Aieta, G. Di Liberto, F. Gabas, R. Conte, and **M. Ceotto***, "Theoretical chemistry and sustainable growth: A trip on board of a nano-engine conducted by Martin Karplus", Nuova Energia **2**, (2016).
20. C. Aieta, F. Gabas, **M. Ceotto***, "An Efficient Computational Approach for the Calculation of the Vibrational Density of States", *J. Phys. Chem. A* **120** (27), 4853-4862 (2016);
21. M. Buchholz, F. Grossmann, **M. Ceotto***, "Mixed semiclassical initial value representation time-averaging propagator for spectroscopic calculations", *J. Chem Phys.*, **144**, 094102 (2016);
22. M. Orlandi, **M. Ceotto***, M. Benaglia*, "Kinetics versus thermodynamics in the proline catalyzed aldol reaction", *Chemical Science* **7** (8), 5421-5427 (2016);
23. L. Rimoldi, C. Ambrosi, G. Di Liberto, L. Lo Presti, **M. Ceotto**, C. Oliva, D. Meroni, S. Cappelli, G. Cappelletti, G. Soliveri, S. Ardizzone, "Impregnation versus Bulk Synthesis: How the Synthetic Route Affects the Photocatalytic Efficiency of Nb/Ta:N Codoped TiO2 Nanomaterials",*J. Phys. Chem C*, **119**, 24104-24115 (2015);

24. F. Spadavecchia*, **M. Ceotto**, L. Lo Presti, C. D. Aieta, I. Biraghi, D. Meroni, S. Ardizzone, G. Cappelletti, "Second Generation Nitrogen Doped Titania Nanoparticles: A Comprehensive Electronic and Microstructural Picture", *Chi. J. of Chemistry*, **32** (12), 1195-1293 (2014);
25. C. Marchiori, G. Di Liberto, G. Soliveri, L. Loconte, L. Lo Presti*, D. Meroni*, **M. Ceotto**, C. Oliva, S. Cappelli, G. Cappelletti, C. Aieta, S. Ardizzone, "Unraveling the Cooperative Mechanism of Visible-light Absorption in Bulk N, Nb Codoped TiO2 Powders of Nanomaterials", *J. Phys. Chem C*, **118**, 24152-24164 (2014);
26. S. Mandrà, J. Schrier, **M. Ceotto***, "Helium Isotope Enrichment by Resonant Tunneling Through Nanoporous Graphene Bilayers" *J. Phys. Chem. A,* **118** (33), 6457-6465 (2014);
27. D. Tamascelli, F.S. Dambrosio, R. Conte, **M. Ceotto***, "Graphics Processing Units Accelerated Semiclassical Initial Value Representation Molecular Dynamics", *J. Chem Phys.*, **140**, 174109 (2014);
28. L. Lo Presti*, **M. Ceotto**, F. Spadavecchia, G. Cappelletti, D. Meroni, R.A. Acres, S. Ardizzone, "Role of the Nitrogen Source in Determining Structure and Morphology of N-Doped Nanocrystalline TiO2", *J. Phys. Chem C*, **118**, 4797-4807 (2014);
29. **M. Ceotto***, C. Manuali, A. Manfredi, "Massive implementation of the European Chemistry Test at University of Milan", Virtual Innovation, Research, Teaching & Learning Communities. - ISSN 2279-8773. - 4 (2013);
30. R. Conte, A. Aspuru-Guzik, **M. Ceotto***, "Reproducing Deep Tunneling Splittings, Resonances, and Quantum Frequencies in Vibrational Spectra From a Handful of Direct Ab Initio Semiclassical Trajectories", *J. Phys. Chem. Lett.*, **4**, 3407−3412 (2013);
31. S. Mandrà, S. Valleau, **M. Ceotto***, "Deep Nuclear Resonant Tunneling Thermal Rate Constant Calculations", *Int. J. of Quantum Chemistry*, **113** (12), 1722-1734 (2013);
32. **M. Ceotto***, Y. Zhuang, W.L. Hase, "Accelerated direct semiclassical molecular dynamics using a compact finite difference Hessian scheme", *J. Chem. Phys.* **138**, 054116 (2013);
33. F. Spadavecchia*, S. Ardizzone, G. Cappelletti, L. Falciola, **M. Ceotto**, D. Lotti, "Investigation and optimization of photocurrent transient measurements on nano-TiO2", *J. of Applied Electrochem.* **43** (2), 217-225 (2013);
34. Y. Zhuang*, M. R. Siebert, W.L. Hase, K.G. Kay, **M. Ceotto***, "Evaluating the Accuracy of Hessian Approximations for Direct Dynamics Simulations" *J. Chem. Theory and Computation*, **9** (1), 54-64 (2013);
35. G. Cappelletti*, S. Ardizzone, D. Meroni, G. Soliveri, **M. Ceotto**, C. Biaggi, M. Benaglia, L. Raimondi, "Wettability of bare and fluorinated silanes: A combined approach based on surface free energy evaluations and dipole moment calculations", *J. of Colloid and Interface Science* **389**, 284-291 (2013);
36. F. Spadavecchia*, G. Cappelletti, S. Ardizzone, **M. Ceotto**, M. S. Azzola, L. Lo Presti, G. Cerrato, L. Falciola, "Role of Pr on the Semiconductor Properties of Nanotitania. An Experimental and First-Principles Investigation", *J. Phys. Chem C* **116** (43), 23083-23093 (2012)
37. **M. Ceotto***, L. Lo Presti*, G. Cappelletti, D. Meroni, F. Spadavecchia, R. Zecca, M. Leoni, P. Scardi, S. Ardizzone, "About the Nitrogen Location in Nanocrystalline N-Doped TiO2: Combined DFT and EXAFS Approach" *J. Chem. Phys. C* **116** (2), 1764-1771, (2012)
38. **M. Ceotto***, "Vibration-assisted tunneling: a semiclassical instanton approach", *Mol. Phy.* **110** (9-19), Special Issue 547-559 (2011)
39. **M. Ceotto***, G.F. Tantardini, A. Aspuru-Guzik, "Fighting the curse of dimensionality in first-principles semiclassical calculations: Non-local reference states for large number of dimensions", *J. Chem. Phys.* **135** (21), 214108 (2011)
40. D. Meroni*, S. Ardizzone, G. Cappelletti, **M. Ceotto**, M. Ratti, R. Annunziata, M. Benaglia, L. Raimondi,"Interplay between Chemistry and Texture in Hydrophobic TiO2 Hybrids", *J. Chem. Phys. C* **115** (38), 18649-18658 (2011);
41. **M. Ceotto***, S. Valleau, G.F. Tantardini, A. Aspuru-Guzik, "First principles semiclassical calculations of vibrational eigenfunctions", *J. Chem. Phys.* **134** (23), 234103 (2011);
42. F. Spadavecchia*, G. Cappelletti, S.Ardizzone, **M. Ceotto**, L. Falciola, "Electronic Structure of Pure and N-Doped TiO2 Nanocrystals by Electrochemical Experiments and First Principles Calculations", *J. Phys. Chem. C* **155** (14), 6381-6391 (2011);
43. D. Meroni*, S. Ardizzone, G. Cappelletti, C. Oliva, **M. Ceotto**, D. Poelman, H. Poelman, "Photocatalytic removal of ethanol and acetaldehyde by N-promoted TiO2 films: The role of the

different nitrogen sources", *Catalysis Today* **161** (1), 169-174 (2011);

44. **M. Ceotto***, D. Dell'Angelo, G.F. Tantardini, "Multiple coherent states semiclassical initial value representation spectra calculations of lateral interactions for CO on Cu(100)", *J. Chem. Phys.* **133** (5), 054701 (2010);
45. **M. Ceotto***, S. Atahan, G. F. Tantardini, A. Aspuru-Guzik, "Multiple coherent states for first-principles semiclassical initial values representation molecular dynamics", *J. Chem. Phys*. **130**, 234113 (2009)
46. **M. Ceotto***, S. Atahan, S. Shim, G. F. Tantardini, A. Aspuru-Guzik, "First-principles semiclassical initial value representation molecular dynamics", *Phys. Chem. Chem. Phys*. **11**, 3861 (2009)
47. **M. Ceotto***, G. F. Tantardini, S. Atahan, A. Aspuru-Guzik, "First-principles implementation of semiclassical initial value representation molecular dynamics", *Multidimensional Quantum Mechanics with Trajectories*, pg.s-8-16, Ed. D. Shalashilin and M. Miranda (CCP6, University of Leeds, 2008) ISBN 978-0-9545289-8-0
48. **M. Ceotto**, G. S. Ayton, G. A. Voth*, "Accelerated Superposition State Molecular Dynamics for Condensed Phase Systems", *J. Chem. Theory Comput.* **4,** 560 (2008).
49. M. Ceotto "Semiclassical and Quantum Instanton approximations for thermal rate constants of chemical reactions", Ph.D. Dissertation Thesis (337 pages), edit by the "University of California at Berkeley" (copyright © 2005 by Michele Ceotto).
50. **M. Ceotto**, S. Yang, W. H. Miller*, "Quantum reaction rate from higher derivatives of the thermal flux-flux autocorrelation function at time zero" *J. Chem. Phys.* **122**, 044109 (2005).
51. **M. Ceotto**, W. H. Miller*, "Test of the quantum instanton approximation for thermal rate constants for some collinear reactions" *J. Chem. Phys.* **120**, 6356 (2004).
52. W. H. Miller*, Y. Zhao, **M. Ceotto**, S. Yang, "Quantum instanton approximation for thermal rate constants of chemical reactions" *J. Chem. Phys.* **119**, 1329 (2003).
53. **M. Ceotto**, A. García-Vela*, "A reduced-dimensionality quantum model which incorporates the full-dimensional energy of the system. Application to the vibrational predissociation of Cl_2-Ne_2" *J. Chem. Phys.* **115**, 2146 (2001).
54. **M. Ceotto**, F. A. Gianturco*, "Internal coordinate couplings and symmetry properties: the search of a conical seam in the protonated oxygen" *J. Phys. Chem. A* **105**, 5197 (2001).
55. **M. Ceotto**, F. A. Gianturco*, "Gas-phase proton affinity of ozone: a computational test of the experimental mechanism" *J. Mol. Struc.-Theochem* **543**, 115 (2001).
56. **M. Ceotto**, F. A. Gianturco*, "Charge-transfer effects in the gas-phase protonation of ozone: locating the conical intersections" *J. Chem. Phys.* **112**, 5820 (2000) 13.
57. **M. Ceotto**, F. A. Gianturco, D. M. Hirst*, "Protonated ozone: structures, energetics and nonadiabatic effects" *J. Phys. Chem. A* 103, 9984 (1999) 48.

ORAL PRESENTATIONS

2019-Feb	Pisa University, Department Seminar (Italy) "*Semiclassical Molecular Dynamics and its Implementation for Spectroscopic Calculations of High Dimensional and Condensed Phase Molecular Systems*", (invited)
2019-Jan	Center for Complexity & Biosystems (University of Milan, Milano), "*Quantum Mechanical Methods for Spectroscopic Calculations of High Dimensional Molecular Systems*" (invited)
2019-Jan	Fifth C4 workshop (Zurich, CH), "*Semiclassical Molecular Dynamics for Spectroscopic Calculations of Complex Systems*", (invited)
2018-Oct	Bochum University, Department Seminar (Germany) "*Semiclassical Methods for Spectroscopic Calculations of High Dimensional Molecular Systems*", (invited)
2017-July	Telluride Intermediate School (CO-USA), Quantum Effects in Condensed Phase Systems, "*Method for Spectroscopic Calculations of High Dimensional Molecular Systems*", (invited)
2017- July	D.E. Shaw Research (Manhattan, New York, USA), internal seminar, "*Semiclassical "Divide-and-Conquer" Method for Spectroscopic Calculations of High Dimensional Molecular Systems*", (invited)
2017-July	XIV International Workshop on Quantum Reactive Scattering, Trieste (IT), "*Quantum and Semiclassical methods for molecular rate constnats and vibrational spectra calculations*",

(invited)

2017-June CECAM-FR-MOSER Discussion Meeting Practical problems with dynamical nuclear quantum effects through semiclassical methods Paris, June 2628, 2017, "*Semiclassical "Divide-and-Conquer" Method for Spectroscopic Calculations of High Dimensional Molecular Systems*", (invited)

2015-Dic. CNR Rome, National Congress of the Italian Chemistry Society, Theoretical and Computational Chemistry division "*A mixed SC-IVR and Thawed Gaussian Propagator*"

2014-Sept. Italian National Chemical Society Meeting (Università della Calabria, Arcavacata di Rende, Italy) "*A General Purpose Implementations of Semiclassical Molecular Dynamics for CPU and GPU hardware*"

2014-Sept. Italian National Chemical Society Meeting (Università della Calabria, Arcavacata di Rende, Italy) "*Doped nano-titania: theoretical insight into structure-property relationships*"

2014-Feb, EPFL Department Seminar (Lausanne, CH) "*A General Purpose Implementations of Semiclassical Molecular Dynamics for CPU and GPU hardware*", (invited)

2014-Jan. Regione Lombardia LISA meeting (Milano, Italy), "*Progettazione di Nuovi Materiali per l'Abbattimento di Inquinanti. Come proteggere i nostri monumenti"*, (invited)

2014-Jan. Max-Planck-Institut fur Physik Komplexer Systeme Department Seminar (Dresden, Germany),*"Ab initio Semiclassical molecular dynamics for CPU and GPU hardware"*, (invited)

2014-Jan. INFN and Consortium GARR Training Workshop on Application Porting (Roma, Italy), *"Introduction to Quantum Espresso for semiconductors applications"*, (invited)

2012-Jul. NSF/PIRE Workshop (Pisa, Italy), *First Principles Semiclassical Molecular Dynamics*, (invited)

2013-Jun. CECAM Workshop "Many-dimensional quantum dynamics with (non)classical trajectories" (Lausanne, Switzerland), "*Ab initio direct semiclassical molecular dynamics*", (invited)

2013-Jun. Italian National Physical Chemical Society Meeting (Alessandria, Italy), "*Doped Titania Nanocrystals explained by Experimental and DFT Characterizations*"

2010-Oct. The 61st Annual Meeting of the International Society of Electrochemistry (Nice, France), "*Doped versus undoped titania nanocrystals: theoretical bottom-up approach vs. experimental flatband potential studies*"

2010-Jul. Istituto Eni Donegani "Transport in Complex Quantum Systems", Novara, Italy "*Resonances in Complex Quantum Systems from a Semiclassical Dynamics Perspective*", (invited)

2010-Feb. EPFL Department Seminar (Lausanne, CH) "*Multiple Coherent States for first-principles Semiclassical Molecular Dynamics*", (invited)

2008-Sept. CCP6 2008 Workshop Multidimensional Quantum Mechanics with Trajectories School of Chemistry,University of Leeds (UK), "*First-principles Semiclassical Molecular Dynamics*", (invited)

2008-Aug. "Quantum Dynamics Concepts: From Path Integrals to Semiclassical" Workshop and Seminar, Max-Planck-Institut fur Physik Komplexer Systeme (Dresden, Germany), "*Semiclassical Initial Value Representation Implementations*", (invited)

2004-Dic. Dipartimento di Chimica dell'Università di Perugia (Italy), "*How to calculate thermal rate constants for chemical reactions*", (invited)

2001-Oct. "Graduate Research Conferente" (GRC), Berkeley (USA); "*How to Mimic Tunnelling from Asymptotic Conditions*"

2000-Mar. Spanish Physical Chemistry Society meeting at Consejo Superior de las Investigaciones Cientifica (CSIC), Madrid (Spain), "*Conical Intersections*", (invited)

1999-Sept. Italian Physical Chemical Society Meeting (Firenze, Italy),"*Conical Intersections effects in the gas phase molecular protonation*"

1999-Jun. Italian Chemical Society Meeting about "Structure, Properties, Reactivity and Dynamics", (Varenna, Italy), "*Conical Intersections effects in the gas phase molecular protonation*"

Milano, June 14th, 2019