ALLEGATO A

UNIVERSITÀ DEGLI STUDI DI MILANO
Procedura di selezione per la chiamata a professore di I fascia da ricoprire ai sensi dell'art. 18, comma 1, della Legge n. 240/2010 per il settore concorsuale _ 03/A2 - MODELLI E METODOLOGIE PER LE SCIENZE CHIMICHE _ , (settore scientifico-disciplinare ___ CHIM/02 - CHIMICA FISICA_____) presso il Dipartimento di _Chimica_____, (avviso bando pubblicato sulla G.U. n. ___18_____ del __07/03/2023_____) - Codice concorso _5255____

Marco Caricato
CURRICULUM VITAE

(N.B. IL CURRICULUM NON DEVE ECCEDERE LE 30 PAGINE E DEVE CONTENERE GLI ELEMENTI CHE IL CANDIDATO RITIENE UTILI AI FINI DELLA VALUTAZIONE.
LE VOCI INSERITE NEL FACSIMILE SONO A TITOLO PURAMENTE ESEMPLIFICATIVO E POSSONO ESSERE SOSTITUITE, MODIFICATE O INTEGRATE)

INFORMAZIONI PERSONALI (NON INSERIRE INDIRIZZO PRIVATO E TELEFONO FISSO O CELLULARE)

COGNOME	CARICATO
NOME	MARCO
DATA DI NASCITA	03/07/1979

TITOLI

TITOLO DI STUDIO
(indicare la Laurea conseguita inserendo titolo, Ateneo, data di conseguimento, ecc.)

Laurea in Chimica
110/110 summa cum laude
31/10/2002
Semiempirical quantum-mechanical models for the study of energies, properties and structures of molecular systems in solution
Università di PISA
Relatori: Prof. Jacopo Tomasi, Prof.ssa Benedetta Mennucci

TITOLO DI DOTTORE DI RICERCA O EQUIVALENTI, OVVERO, PER I SETTORI INTERESSATI, DEL DIPLOMA DI SPECIALIZZAZIONE MEDICA O EQUIVALENTE, CONSEGUITO IN ITALIA O ALL'ESTERO
(inserire titolo, ente, data di conseguimento, ecc.)

Dottore di ricerca in chimica teorica e computazionale
70/70 summa cum laude
Theoretical models to describe time-dependent and nonequilibrium solvation
Scuola Normale Superiore di PISA
Relatore: Prof. Jacopo Tomasi

ALTRI TITOLI CONSEGUITI
(inserire titolo, ente, data di conseguimento, ecc.)

Associate Professor
University of Kansas
18/08/2019 – oggi
(Il titolo di Full Professor sarà effettivo dall'inizio del prossimo anno accademico, agosto 2023)

Assistant Professor
University of Kansas
18/08/2014 - 17/08/2019

Research Scientist
Gaussian, Inc. (USA)
01/04/2010 – 17/08/2014

Postdoctoral Fellow
Yale University
01/03/2006 - 31/03/2010

ATTIVITÀ DIDATTICA

INSEGNAMENTI E MODULI
(inserire periodo [gg/mm/aa inizio e fine], anno accademico, corso laurea, numero di ore frontali, eventuale CFU)

- Docente del corso di dottorato in chimica: *Introduzione alla meccanica quantistica*.
  Department of Chemistry, University of Kansas. 3 ore frontali a settimana.
  CHEM 750 (Graduate Introduction to Quantum Mechanics), Fall Semester 2014.
  25/08/2014 - 19/12/2014
- Docente del corso di dottorato in chimica. Titolo: *Meccanica quantistica avanzata*.
  Department of Chemistry, University of Kansas. 3 ore frontali a settimana.
  CHEM 850 (Graduate Advanced Quantum Mechanics), Spring Semester 2015.
  20/01/2015 - 15/05/2015
- Docente del corso di dottorato in chimica: *Introduzione alla meccanica quantistica*.
  Department of Chemistry, University of Kansas. 3 ore frontali a settimana.
  CHEM 750 (Graduate Introduction to Quantum Mechanics), Fall Semester 2015.
  24/08/2015 - 18/12/2015
- Docente del corso di laurea in chimica: *Chimica Fisica II, Termodinamica, Meccanica Statistica e Cinetica*.
  Department of Chemistry, University of Kansas. 3 ore frontali a settimana.
  CHEM 535 (Undergraduate Physical Chemistry II), Spring Semester 2016.
  19/01/2016 - 13/05/2016
- Docente del corso di laurea in chimica: *Chimica Fisica I, Meccanica Quantistica*.
  Department of Chemistry, University of Kansas. 4 ore frontali a settimana.
  CHEM 530 (Undergraduate Physical Chemistry I), Fall Semester 2016.
  21/08/2016 - 16/12/2016
- Docente del corso di laurea in chimica: *Chimica Fisica I, Meccanica Quantistica*.
  Department of Chemistry, University of Kansas. 4 ore frontali a settimana.
  CHEM 530 (Undergraduate Physical Chemistry I), Fall Semester 2017.
  21/08/2017 - 15/12/2017
- Docente del corso di laurea in chimica: *Chimica Fisica II, Termodinamica, Meccanica Statistica e Cinetica*.
  Department of Chemistry, University of Kansas. 3 ore frontali a settimana.
  CHEM 535 (Undergraduate Physical Chemistry II), Spring Semester 2018.
  16/01/2018 - 11/05/2018
- Docente del corso di laurea in chimica: *Chimica Fisica I, Meccanica Quantistica*.
  Department of Chemistry, University of Kansas. 4 ore frontali a settimana.
  CHEM 530 (Undergraduate Physical Chemistry I), Fall Semester 2018.
  20/08/2018 - 14/12/2018

- Docente del corso di laurea in chimica: *Chimica Fisica II, Termodinamica, Meccanica Statistica e Cinetica*.
  Department of Chemistry, University of Kansas. 3 ore frontali a settimana.
  CHEM 535 (Undergraduate Physical Chemistry II), Spring Semester 2019.
  22/01/2019 - 17/05/2019
- Docente del corso di dottorato in chimica: *Introduzione alla meccanica quantistica*.
  Department of Chemistry, University of Kansas. 3 ore frontali a settimana.
  CHEM 750 (Graduate Introduction to Quantum Mechanics), Fall Semester 2019.
  26/08/2019 - 20/12/2019
- Docente del corso di laurea in chimica: *Metodi matematici per scienze chimiche*.
  Department of Chemistry, University of Kansas. 3 ore frontali a settimana.
  CHEM 250 (Undergraduate Mathematical Methods for Chemical Sciences), Spring Semester 2020.
  21/01/2020 - 15/05/2020
- Docente del corso di dottorato in chimica. Titolo del corso*: Meccanica quantistica avanzata.*
  Department of Chemistry, University of Kansas. 3 ore frontali a settimana.
  CHEM 850 (Graduate Advanced Quantum Mechanics), Fall Semester 2021.
  23/08/2021 - 17/12/2021
- Docente del corso di laurea in chimica: *Metodi matematici per scienze chimiche*.
  Department of Chemistry, University of Kansas. 3 ore frontali a settimana.
  CHEM 250 (Undergraduate Mathematical Methods for Chemical Sciences), Spring Semester 2022.
  18/01/2022 - 13/05/2022
- Docente del corso di dottorato in chimica. Titolo del corso: *Spectroscopia molecolare*.
  Department of Chemistry, University of Kansas. 3 ore frontali a settimana.
  Denominazione corso: CHEM 856 (Graduate Molecular Spectroscopy), Fall Semester 2022.
  21/08/2022 - 12/09/2022
- Docente del corso di laurea in chimica: *Metodi matematici per scienze chimiche*.
  Department of Chemistry, University of Kansas. 3 ore frontali a settimana.
  CHEM 250 (Undergraduate Mathematical Methods for Chemical Sciences), Spring Semester 2023.
  17/01/2023 - 05/05/2023

ATTIVITÀ DI DIDATTICA INTEGRATIVA E DI SERVIZIO AGLI STUDENTI

ATTIVITÀ DI RELATORE DI ELABORATI DI LAUREA, DI TESI DI LAUREA MAGISTRALE, DI TESI DI DOTTORATO E DI TESI DI SPECIALIZZAZIONE

(inserire numero, anno accademico, ateneo, corso laurea, ecc.)

Relatore tesi di dottorato in chimica alla University of Kansas (PhD):
- K. Zhang (12/12/2022), ora Postdoc al CNRS, Francia
- T. Balduf (29/03/2022), ora Research Scientist da Schrodinger, Inc., USA
- S. Ren (29/05/2020), ora Postdoc alla Northeastern University, USA
- A. Jystad (05/06/2020), ora Postdoc al PNNL, USA
- M. Barclay (13/12/2019), ora Postdoc a Boise State University, USA
- T. Aharon (30/08/2019), ora Data Architect da TetraScience, USA

Relatore tesi di laurea magistrale alla University of Kansas (MS):
- I. Moore (26/04/2022)

Nota: negli USA, gli studenti del corso di laurea non difendono una tesi per laurearsi, ma la laurea è conseguita al completamento dei corsi previsti dal dipartimento. Gli studenti del corso di laurea possono comunque fare ricerca come undergraduate research assistants (UGRAs).
Il corso di dottorato (PhD) dura 5 anni e si conclude con una tesi. Il corso di PhD include al terzo anno un esame equivalente alla laurea magistrale come passo intermedio, ma il diploma di laura magistrale non viene riportato a meno che lo studente non si fermi a quel punto. Alla University of Kansas, questo esame (comprehensive oral exam) prevede la scrittura e la difesa di un progetto di ricerca diverso da quello condotto dallo studente nel proprio gruppo di ricerca.

ATTIVITÀ DI TUTORATO DEGLI STUDENTI DI CORSI DI LAUREA E DI LAUREA MAGISTRALE E DI TUTORATO DI DOTTORANDI DI RICERCA
(inserire anno accademico, corso laurea, ecc.)

Studenti di dottorato in chimica attualmente nel mio gruppo:
- T. Parsons, 3° anno (data prevista di termine del dottorato: 2025)
- S. Brahmachari, 1° anno (data prevista di termine del dottorato: 2027)
- E. Forson, 1° anno (data prevista di termine del dottorato: 2027)

Studenti del corso di laurea in chimica attualmente nel mio gruppo come *undergraduate research assistants* (UGRAs):
- S. Haenggi
- B. Faintich
- J. Osborn
- E. Brenneman
- A. Dowson

Dall'inizio della mia carriera accademica, 16 UGRAs (compresi i presenti) hanno fatto ricerca nel mio gruppo.

Studenti di scuola superiore attualmente nel mio gruppo come *research volunteers*:
- I. Li
- J. Wiltanger

Dall'inizio della mia carriera accademica, 4 studenti di scuola superiore (compresi i presenti) hanno fatto ricerca nel mio gruppo.

Ho fatto parte di oltre 10 commissioni di dottorato and oltre 15 commissioni per il comprehensive oral exam del terzo anno del corso di dottorato (oltre a quelle dei miei studenti).

ATTIVITÀ DI RICERCA SCIENTIFICA

PUBBLICAZIONI SCIENTIFICHE
(per ciascuna pubblicazione indicare: nomi degli autori, titolo completo, casa editrice, data e luogo di pubblicazione, codice ISBN, ISSN, DOI o altro equivalente)

* Corresponding Author

1. Articolo in rivista
   Zhang Kaihua, Caricato Marco* (2023). Modeling Catalyzed Reactions on Metal-Doped Amorphous Silicates: The Case of Niobium-Catalyzed Ethylene Epoxidation, JOURNAL OF PHYSICAL CHEMISTRY C, 127, 4984, doi: 10.1021/acs.jpcc.3c00213.
   Journal cover: https://pubs.acs.org/toc/jpccck/127/10
2. Articolo in rivista
   Balduf Ty*, Caricato Marco* (2022). Derivation and implementation of the optical rotation tensor for chiral crystals. JOURNAL OF CHEMICAL PHYSICS, 157, 214105, doi: 10.1063/5.0130385
3. Articolo in rivista
   Zhang Kaihua, Balduf Ty, Caricato Marco* (2021) Full optical rotation tensor at coupled cluster with single and double excitations level in the modified velocity gauge. CHIRALITY, 33, 303, doi: 10.1002/chir.23310
4. Articolo in rivista
   Vandervelden Craig, Jystad Amy, Peters Baron*, Caricato Marco* (2021). Predicted Properties of Active Catalyst Sites on Amorphous Silica: Impact of Silica Preoptimization Protocol. INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH, 60, 12834, doi: 10.1021/acs.iecr.1c01849
5. Articolo in rivista
   Caricato Marco* (2021). Cluster Model Simulations of Metal-Doped Amorphous Silicates for Heterogeneous Catalysis. JOURNAL OF PHYSICAL CHEMISTRY C, 125, 27509, doi: 10.1021/acs.jpcc.1c07524. Journal cover: https://pubs.acs.org/toc/jpccck/125/50
6. Articolo in rivista
   Caricato Marco* (2020). Coupled cluster theory in the condensed phase within the singles-T density

scheme for the environment response. WILEY INTERDISCIPLINARY REVIEWS. COMPUTATIONAL MOLECULAR SCIENCE, e1463, doi: 10.1002/wcms.1463

7. Articolo in rivista
   Barclay Matthew S., Elles Christopher G.*, Caricato Marco* (2020). On the Discrepancy between Experimental and Calculated Raman Intensities for Conjugated Phenyl and Thiophene Derivatives. JOURNAL OF PHYSICAL CHEMISTRY A, 124, 4678, doi: 10.1021/acs.jpca.0c00363
8. Articolo in rivista
   Caricato Marco* (2020). Origin invariant optical rotation in the length dipole gauge without London atomic orbitals. JOURNAL OF CHEMICAL PHYSICS, 153, 151101, doi: 10.1063/5.0028849
9. Articolo in rivista
   Caricato, Marco* (2019) CCSD-PCM Excited State Energy Gradients with the Linear Response Singles Approximation to Study the Photochemistry of Molecules in Solution. CHEMPHOTOCHEM, 3, 2367, doi: 10.1002/cptc.201900152.
10. Articolo in rivista
    Ren Sijin, Lipparini Filippo, Mennucci Benedetta, Caricato Marco* (2019). Coupled Cluster Theory with Induced Dipole Polarizable Embedding for Ground and Excited States. JOURNAL OF CHEMICAL THEORY AND COMPUTATION, 15, 4485, doi: 10.1021/acs.jctc.9b00468
11. Articolo in rivista
    DeLucia Nicholas A., Jystad Amy, Vander Laan Katherine, Tengco John Meynard M., Caricato Marco*, Vannucci Aaron K.* (2019). Silica Supported Molecular Palladium Catalyst for Selective Hydrodeoxygenation of Aromatic Compounds under Mild Conditions. ACS CATALYSIS, 9, 9060, doi: 10.1021/acscatal.9b02460
12. Articolo in rivista
    Jystad Amy, Caricato Marco* (2018). Computational Multinuclear NMR Characterization of Metal-Doped Amorphous Silica Catalysts. CHEMISTRY OF MATERIALS, 30, 7813, doi: 10.1021/acs.chemmater.8b03257
13. Articolo in rivista
    Jystad Amy M., Biancardi Alessandro, Caricato Marco* (2017). Simulations of Ammonia Adsorption for the Characterization of Acid Sites in Metal-Doped Amorphous Silicates. JOURNAL OF PHYSICAL CHEMISTRY C, 121, 22258, doi: 10.1021/acs.jpcc.7b08113
14. Articolo in rivista
    Biancardi Alessandro, Caraiani Claudiu, Chan Wai-Lun, Caricato Marco* (2017). How the Number of Layers and Relative Position Modulate the Interlayer Electron Transfer in π-Stacked 2D Materials. JOURNAL OF PHYSICAL CHEMISTRY LETTERS, 8, 1365, doi: 10.1021/acs.jpclett.7b00194
15. Articolo in rivista
    Barclay Matthew S., Quincy Timothy J., Williams-Young David B., Caricato Marco*, Elles Christopher G.* (2017). Accurate Assignments of Excited-State Resonance Raman Spectra: A Benchmark Study Combining Experiment and Theory. JOURNAL OF PHYSICAL CHEMISTRY A, 121, 7937, doi: 10.1021/acs.jpca.7b09467
16. Articolo in rivista
    Ren Sijin, Caricato Marco* (2016). Multi-state extrapolation of UV/Vis absorption spectra with QM/QM hybrid methods. JOURNAL OF CHEMICAL PHYSICS, 144, 184102, doi: 10.1063/1.4948471
17. Articolo in rivista
    Caricato Marco*, Curutchet Carles, Mennucci Benedetta, Scalmani Giovanni (2015). Electronic Couplings for Resonance Energy Transfer from CCSD Calculations: From Isolated to Solvated Systems. JOURNAL OF CHEMICAL THEORY AND COMPUTATION, 11, 5219, doi: 10.1021/acs.jctc.5b00720
18. Articolo in rivista
    Caricato Marco* (2015). Orbital Analysis of Molecular Optical Activity Based on Configuration Rotatory Strength. JOURNAL OF CHEMICAL THEORY AND COMPUTATION, 11, 1349, doi: 10.1021/acs.jctc.5b00051
19. Articolo in rivista
    Caricato Marco* (2013). A comparison between state-specific and linear-response formalisms for the calculation of vertical electronic transition energy in solution with the CCSD-PCM method. JOURNAL OF CHEMICAL PHYSICS, 139, 044116, doi: 10.1063/1.4816482
20. Articolo in rivista
    Caricato Marco* (2012). Absorption and Emission Spectra of Solvated Molecules with the EOM–CCSD–PCM Method. JOURNAL OF CHEMICAL THEORY AND COMPUTATION, 8, 4494, doi: 10.1021/ct3006997

ORGANIZZAZIONE, DIREZIONE E COORDINAMENTO DI CENTRI O GRUPPI DI RICERCA NAZIONALI E INTERNAZIONALI O PARTECIPAZIONE AGLI STESSI
(per ciascuna voce inserire anno, ruolo, gruppo di ricerca, ecc.)

- Progetto finanziato dalla National Science Foundation, USA:
  M. Caricato. Periodic Coupled Cluster Methods for Optical Activity in Chiral Crystals. National Science Foundation, $456,483. 05/01/2022 - 04/30/2025.

- Progetto finanziato dal Department of Energy, USA:
  M. Caricato (Principal Investigator), Co-Principal: B. B. Laird, B. Peters, W. H. Thompson. Ab Initio Ma- chine Learning Algorithms for Modeling Kinetics on Amorphous Catalysts. Department of Energy, $1,588,000. 09/15/2018 - 09/14/2023.

- Progetto finanziato dalla National Science Foundation, USA:
  M. Caricato. First Principles Evaluation of Optical Activity in Solids. National Science Foundation CAREER, $625,000. 04/01/2017 - 06/30/2023.

- Progetto finanziato dalla National Science Foundation, USA:
  Principal Investigators: B. Subramaniam, J. Regalbuto, Co-Principal: J. Bravo Suárez, M. Caricato, F. Tao, R. V. Chaudhari, M. Yu, V. Aaron. RII Track-2 FEC: Catalysis for Renewables: Applications, Fundamentals and Technologies (CRAFT). National Science Foundation, $4,000,000. 08/01/2015 - 07/31/2019.

- Progetto finanziato dalla National Science Foundation, USA:
  M. Caricato. Multilayer Strategies for the Investigation of Electron Recombination Reactions in Organic Photovoltaics. EPS-0903806, Kansas NSF EPSCoR, $84,486. 01/01/2015 - 09/30/2015.

ATTIVITÀ QUALI LA DIREZIONE O LA PARTECIPAZIONE A COMITATI EDITORIALI DI RIVISTE SCIENTIFICHE
(per ciascuna voce inserire anno, ruolo, rivista scientifica, ecc.)

Membro della Editorial Advisory Board:
- Chirality, Wiley, 2019-oggi
- Journal of Physical Chemistry A/B/C, American Chemical Society, 2023 - oggi

PREMI E RICONOSCIMENTI NAZIONALI E INTERNAZIONALI PER ATTIVITÀ DI RICERCA
(inserire premio, data, ente organizzatore, ecc.)

- Kansas EPSCoR First Award 2015
  Descrizione:
  The First Award program helps early career faculty become more competitive for funding from the research directorates at the National Science Foundation (NSF) by 1) encouraging early career faculty to submit proposals to the NSF (or other federal funding agency) as soon as possible after their first faculty appointment, and 2) by accelerating the pace of their research and the quality of their subsequent proposals. First Awards are intended to be single-investigator awards to support the PI's research program at their institution.

- NSF CAREER Award 2017
  Descrizione:
  The National Science Foundation CAREER awards are the National Science Foundation's most prestigious awards in support of junior faculty who exemplify the role of teacher-scholars through research, education and the integration of education and research within the context of the mission of their organizations. The award comes with a federal grant for research and education activities for five consecutive years. NSF grants these awards once a year. The reviewing, award and selection process is one of the most competitive within the NSF. NSF CAREER awards support promising and talented researchers in building a foundation for a lifetime of leadership in integrating education and research.

- ACS COMP OpenEye Outstanding Junior Faculty Award - ACS 2019
  Descrizione:
  The ACS COMP OpenEye Outstanding Junior Faculty Award program provides $1,000 to up to four outstanding tenure-track junior faculty members to present their work in COMP division at the ACS National Meeting. The Awards are designed to assist new faculty members in gaining visibility within the COMP community. Award certificates and $1,000 prizes will be presented. Applications for Outstanding Junior Faculty Awards are invited from all current tenure-track junior (untenured) faculty who are members of ACS and the ACS Division of Computers in Chemistry.

- I&EC Research's 2021 Class of Influential Researchers Award
  Descrizione:
  Industrial & Engineering Chemistry Research is delighted to announce the 2021 Class of Influential Researchers. These talented researchers, who are in the first 10 years or so of their independent careers, were identified through an open call for nominations, with a focus on researchers in the Americas. The nominations were then reviewed by our global team of editors and advisory board members and selected based on the quality and impact of their research.

PARTECIPAZIONE IN QUALITÀ DI RELATORE A CONGRESSI E CONVEGNI DI INTERESSE INTERNAZIONALE
(inserire titolo congresso/convegno, data, ecc.)

Seminari su Invito a Congressi Internazionali:

1. Fall ACS National Meeting, Chicago, IL, August 22, 2022: Simulations of Resonance-Enhanced Femtosecond Stimulated Raman Spectroscopy.
2. 18th International Conference on Chiroptical Spectroscopy, New York City, NY, July 25, 2022: First Principles Simulations of the Optical Rotation in Oriented Systems with Periodic Density Functional Theory.
3. Great Plains Catalysis Society Webinar Series, July 30, 2021: Quantum Chemistry Simulations of Heterogenous Catalysis on Amorphous Silicates.
4. ACS National Meeting, San Diego, CA, August 27, 2019: Computational Catalysis on Amorphous Silicates.
5. DOE CTC/CCS PI Meeting, Gaithersburg, MD, May 22, 2019: Ab Initio Machine Learning Algorithms for Modeling Kinetics on Amorphous Catalysts.
6. ACS National Meeting, Orlando, FL, April 4, 2019: Multi-State QM/QM Extrapolation with Electronic Embedding for Excitation Energies.
7. TAMUQ meeting, Doha, Qatar, March 3, 2019: Computational Catalysis on Amorphous Silicates.
8. JACC 2018, Noirmoutier, France, September 26, 2018: Orbital Analysis of the Optical Rotation in Helicenes.
9. ACS Midwest Regional Meeting, Lawrence, KS, October 19, 2017: Theoretical Characterization of Metal-Doped Amorphous Silicates.
10. ACS National Meeting, San Diego, CA, March 16, 2016: Computational Investigation of Lewis and Brønsted Acidity in Metal-Doped Mesoporous Silicates.
11. ACS National Meeting, San Diego, CA, March 13 2016: Evaluation of Electronic Coupling in Solids with DFT and PBC Calculations.
12. Solutions for Solvation Workshop, Pisa, Italy, September 1, 2014: Coupled Cluster Calculations of Excited State Properties in Solution.
13. TSRC Excited States and Time-Dependent Electronic Structure Theory, Telluride CO, July 14, 2014: Exploring Excited States in Solution with Coupled Cluster and Polarizable Solvation Methods Spectra in Solution.
14. TSRC Electronic and Magnetic Properties of Chiral Structures and their Assemblies, Telluride CO, July 1, 2014: Insights on the Origin of the Unusually Large Specific Rotation of (1S, 4S)-Norbornenone.
15. SERMACS 2013 meeting, Atlanta GE, November 14, 2013: Towards the Accurate Simulation of UV/Vis Spectra in Solution.
16. ACS National meeting, Philadelphia PA, August 19-23, 2012: State specific EOM-CCSD-PCM method for exploring potential energy surfaces of electronic excited states in solution.

Seminari su Contributo a Congressi Internazionali:

1. Spring ACS National Meeting, Indianapolis, IN, March 28, 2023: Modeling catalyzed reactions on metal-doped amorphous silicates: The case of niobium-catalyzed ethylene epoxidation.

2. Spring ACS National Meeting, San Diego, CA, March 23, 2022: Origin Invariant Optical Rotation Tensor in the Length Dipole Gauge without London Atomic Orbitals.
3. Spring ACS National Meeting, San Diego, CA, March 20, 2022: Predicted Properties of Active Catalyst Sites on Amorphous Silica: Impact of Silica Preoptimization Protocol.
4. Pacifichem, Virtual, December 18, 2021: Origin Invariant Optical Rotation Tensor in the Length Dipole Gauge without London Atomic Orbitals.
5. Pacifichem, Virtual, December 18, 2021: Surface Acidity Characterization of Metal-Doped Amorphous Silicates via Py-FTIR and 15N NMR Simulations.
6. Pacifichem, Virtual, December 18, 2021: CCSD-PCM excited state energy gradients with the linear response singles approximation to study the photochemistry of molecules in solution.
7. APS March Meeting, Virtual, March 16, 2021: Origin Invariant Optical Rotation Tensor in the Length Dipole Gauge without London Atomic Orbitals.
8. AIChE National Meeting, Virtual, November 17, 2020: Surface Acidity Characterization of Metal-Doped Amorphous Silicates via Py-FTIR and ^{15}N NMR Simulations.
9. NSF 26th EPSCoR National Conference, Columbia, SC, October 27-30, 2019: Silica Supported Molecular Pd Catalyst for Selective Hydrodeoxygenation of Aromatic Compounds. Selected for Lightning Talk.
10. CD 2019, Pisa, Italy, June 23-27, 2019: Configuration Space Analysis of the Specific Rotation of Helicenes.
11. PPES 2018, Pisa, Italy, June 24-27, 2018: Electronic Coupling for Donor-Bridge-Acceptor Systems with a Bridge-Overlap Approach.
12. CD2017, Rennes, France, June 11-15, 2017: Investigation of Solvation Effects on Optical Rotatory Dispersion using the Polarizable Continuum Model.
13. APS March Meeting 2017, New Orleans, LA, March 13-17, 2017: How Number of Layers and Relative Position Modulate the Interlayer Electron Transfer in π-Stacked 2D Materials.
14. 2016 AIChE National Meeting, San Francisco, CA, November 13-18, 2016: Computational Investigation of Lewis and Brønsted Acidity In Metal-Doped Mesoporous Silicates.
15. TACC 2016, Seattle, WA, August 28-September 2, 2016: Efficient CC-PCM Methods for Excited States and Response Properties.
16. Pacifichem 2015, Honolulu, HI, December 15-20, 2015: Orbital Analysis of Molecular Optical Activity Based on Configuration Rotatory Strength.
17. 15th International Conference on Chiroptical Spectroscopy, Sapporo, Japan, August 30-September 3, 2015: Orbital Analysis of Molecular Optical Activity Based on Configuration Rotatory Strength.
18. ACS National meeting, Boston MA, August 16-20, 2015: Computational screening of possible brown carbon compounds in the atmospheric aerosol.
19. ACS National meeting, Boston MA, August 16-20, 2015: Orbital Analysis of Molecular Optical Activity Based on Configuration Rotatory Strength.
20. Chirality 2015, Boston MA, June 28-July 1, 2015: Orbital Analysis of Molecular Optical Activity Based on Configuration Rotatory Strength.
21. ACS National meeting, Denver CO, March 22-26, 2015: How Reliable Are Calculations of Absorption Spectra of Solvated Molecules with CC Theory and PCM?
22. WATOC 2014, Santiago, Chile, October 6, 2014: Benchmarking Calculations of Electronic Energy Transfer Coupling in Gas Phase and in Solution.

Seminari su Invito a Dipartimenti Universitari e National Laboratories:

1. University of California Merced, Merced, CA, December 2nd, 2022: First Principles Simulations of the Optical Rotation in Oriented Systems with Periodic Density Functional Theory.
2. University of Missouri, Columbia, MO, October 14th, 2022: First Principles Simulations of the Optical Rotation in Oriented Systems with Periodic Density Functional Theory.
3. Scuola Normale Superiore, Pisa, Italy, June 28, 2022: First Principles Simulations of the Optical Rotation in Oriented Systems with Periodic Density Functional Theory.
4. Scuola Normale Superiore, Pisa, Italy, June 27, 2018: Characterization of Structural and Electronic Properties of Materials from a Molecular Electronic Structure Theory Perspective.
5. University of Washington, Seattle, WA, April 18, 2018: Characterization of Structural and Electronic Properties of Materials from a Molecular Electronic Structure Theory Perspective.
6. Washington State University, Pullman, WA, April 16, 2018: Characterization of Structural and Electronic Properties of Materials from a Molecular Electronic Structure Theory Perspective.
7. Wayne State University, Detroit, MI, April 11, 2018: Characterization of Structural and Electronic Properties of Materials from a Molecular Electronic Structure Theory Perspective.

8. Michigan State University, Lansing, MI, April 10, 2018: Characterization of Structural and Electronic Properties of Materials from a Molecular Electronic Structure Theory Perspective.
9. Kansas State University, Manhattan, KS, April 5, 2018: Characterization of Structural and Electronic Properties of Materials from a Molecular Electronic Structure Theory Perspective.
10. Indiana University, Bloomington, IN, March 29, 2018: Characterization of Structural and Electronic Properties of Materials from a Molecular Electronic Structure Theory Perspective.
11. Purdue University, West Lafayette, IN, March 28, 2018: Characterization of Structural and Electronic Properties of Materials from a Molecular Electronic Structure Theory Perspective.
12. Rutgers University, New Brunswick, NJ, February 9, 2018: Characterization of Structural and Electronic Properties of Materials from a Molecular Electronic Structure Theory Perspective.
13. Rutgers University, Newark, NJ, February 8, 2018: Characterization of Structural and Electronic Properties of Materials from a Molecular Electronic Structure Theory Perspective.
14. Yale University, New Haven, CT, February 7, 2018: Characterization of Structural and Electronic Properties of Materials from a Molecular Electronic Structure Theory Perspective.
15. New York University, New York, NY, February 6, 2018: Characterization of Structural and Electronic Properties of Materials from a Molecular Electronic Structure Theory Perspective.
16. Virginia Tech, Blacksburg, VA, February 2, 2018: Characterization of Structural and Electronic Properties of Materials from a Molecular Electronic Structure Theory Perspective.
17. SUNY Buffalo, Buffalo, NY, December 6, 2017: Characterization of Structural and Electronic Properties of Materials from a Molecular Electronic Structure Theory Perspective.
18. Université d'Angers, Angers, France, June 16, 2017: Insights on the Optical Rotation of Chiral Molecules from Quantum Mechanical Simulations.
19. Emerging Feedstock Forum, University of Kansas, Lawrence, KS, May 3, 2016: Driving Catalytic Innovations with Computational Chemistry.
20. Kansas Physical Chemistry Symposium, Kansas State University, Manhattan KS, October 18, 2014: Coupled Cluster Calculations of Excited State Properties in Solution.
21. Physics Colloquium, Department of Physics at KU, Lawrence KS, September 15, 2014: Coupled Cluster Calculations of Excited State Properties in Solution.
22. DyMERS Seminar, Department of Chemistry at KU, Lawrence KS, September 10 Coupled Cluster Calculations of Excited State Properties in Solution.
23. Scuola Normale Superiore, Pisa Italy, October 24, 2013: Towards the Accurate Simulation of UV/Vis Spectra in Solution.
24. Indiana University, Bloomington IN, September 13, 2013: Towards the Accurate Simulation of Excited States Properties in Solution through the Combination of CCSD and Polarizable Solvation Models.
25. University of Washington, Seattle WA, August 23, 2013: Towards the Accurate Simulation of Excited States Properties in Solution through the Combination of CCSD and Polarizable Solvation Models.
26. Pacific Northwest National Laboratory, Richland WA, August 20, 2013: Towards the Accurate Simulation of UV/Vis Spectra in Solution.

ATTIVITÀ GESTIONALI, ORGANIZZATIVE E DI SERVIZIO

INCARICHI DI GESTIONE E AD IMPEGNI ASSUNTI IN ORGANI COLLEGIALI E COMMISSIONI, PRESSO RILEVANTI ENTI PUBBLICI E PRIVATI E ORGANIZZAZIONI SCIENTIFICHE E CULTURALI, OVVERO PRESSO L'ATENEO O ALTRI ATENEI

(inserire incarico/impegno, ente, data, ecc.)

Attività Professionali in Organizzazioni Scientifiche

Appartenenza a Organizzazioni Scientifiche:

- American Chemical Society (ACS): 2006 – oggi
- American Physical Society (APS): 2012 – oggi
- American Association for the Advancement of Science (AAAS): 2018 - oggi

Appartenenza a Comitati Esecutivi:

- Member at-Large dell'Executive Committee della divisione PHYS dell'ACS.

Organizzazione di simposi e workshop internazionali:

- QM/QM and Embedding Models at the Spring 2023 ACS National Meeting, Indianapolis, IN, 26-30 March 2023, coorganized with L. Slipchenko (Purdue U.).
- New Developments in Hybrid QM/QM, QM/MM, and Fragmentation Methods at the Spring 2022 ACS National Meeting, San Diego, CA, 20- 24 March 2022, coorganized with J. Herbert (Ohio State U.).
- ACS PHYS division monthly webinars, 08/2021–02/2022, coorganized with R. Noriega (U. Utah), V. Huxton (U. Arizona), L. Wang (Rutgers U.).
- Chirality from Molecules to Materials Symposium at the 255th ACS National Meeting, New Orleans, LA, 18-22 March 2018, coorganized with P. H. Vaccaro (Yale U.).
- Physical Chemistry Symposium at the 2017 Midwest Regional Meeting of the ACS, Lawrence, KS, October 18-20, 2017.
- MolSSI's Coding Solvation Workshop, Livorno (Italy) August 23-25 2017, coorganized with L. Frediani (UiT), H. Kulik (MIT), B. Mennucci (U. Pisa), R. Di Remigio (UiT), O. Andreussi (UNT), M. Olsen (DTU), and F. Lipparini (U. Pisa).

Attività Professionali come Proposal Reviewer:

- Membro del Panel Review per la National Science Foundation, 2023
- Membro del Panel Review per la National Science Foundation, 2020
- Ad-Hoc Proposal Reviewer per il Department of Energy, 2018-2022
- Ad-Hoc Proposal Reviewer per lo European Research Council, 2017
- Ad-Hoc Proposal Reviewer per il Pertroleum Research Fund ACS, 2015 e 2018
- Ad-Hoc Proposal Reviewer per la fondazione Lumomat (Francia), 2018

Attività Professionali come Journal Reviewer:

ACIE, ACS Books, ACS Sustain. Chem. Eng., Chem. Data Collect., Chem. Phys. Lett., ChemPhysChem, Comput. Theor. Chem., Int. J. Quantum Chem., J. Chem. Phys., J. Chem. Theory Comput., J. Comput. Chem., J. Lumin., J. Phys. Chem. A/B/C/Lett, J. Am. Chem. Soc., Molecules, Mol. Phys., Phys. Chem. Chem. Phys., RSC Advances, Spectrochim. Acta, Theor. Chem. Acc.

Servizio Accademico alla University of Kansas

Commissioni a livello di Dipartimento:

- Direttore del Graduate Admission Committee (2022-2023)
- Direttore del Faculty Review Committee (2021-2022)
- Membro del Graduate Admission Committee (2015-2018, 2021-2022)
- Membro del Graduate Recruiting Committee (2014-2015).
- Membro del Chair Advisory Committee (2014-2015, 2017-2018, 2019-2020).
- Membro del Faculty Review Committee (2019-2022).

Commissioni a livello di Facoltà (College of Liberal Arts and Sciences):

- Direttore del College Committee on Graduate Studies (2022-2023)
- Membro del College Committee on Graduate Studies (2020 -2023)

Commissioni a livello di Università:

- Membro del Research Technology Workgroup (2021)

Servizio Accademico al di fuori della University of Kansas:

- Revisore esterno della Tesi di Perfezionamento (dottorato) per la Scuola Normale Superiore di Pisa, 2022.
- Membro del Collegio dei Docenti del Corso di Perfezionamento "Metodi e modelli per le scienze molecolari" della Scuola Normale Superiore di Pisa, 2022 - oggi.

Data 31/03/2023 Luogo Lawrence, KS, USA