Umberto Raucci - Resume

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Research Interests

ab initio molecular dynamics, nonadiabatic molecular dynamics, QM/MM, photochemistry, mechanochemistry, reaction discovery, neural network potentials, heterogeneous catalysis, natural user interfaces for quantum chemistry

Research Experience

2021-present	**Postdoctoral Researcher** - Advisor: Prof. Michele Parrinello *Italian Institute of Technology*, Genova, Italy
2019-2021	**Postdoctoral Researcher** - Advisor: Prof. Todd J. Martínez *Stanford University*, CA, USA
10/2018-12/2018	**Postdoctoral Researcher** - Advisor: Prof. Carlo Adamo *Chimie ParisTech, PSL University* collaboration with *L'Oréal Paris*, Paris, France
2016-2018	**Postdoctoral Researcher** - Advisor: Prof. Nadia Rega *University of Naples Federico II*, Naples, Italy
05/2015-07/2015	**Visiting Student** - Advisor: Prof. Carlo Adamo *Chimie ParisTech, PSL University*, Paris, France

Academic Education

2013-2016	**PhD in Chemical Sciences** *University of Naples Federico II*, Naples, Italy
2009-2012	**Master in Chemical Sciences** (110/110) *University of Naples Federico II*, Naples, Italy
2006-2009	**Bachelor in Chemistry** (summa cum laude) *University of Naples Federico II*, Naples, Italy

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Participation in workshops and training courses

2022	*PyTorch for Deep Learning with Python Bootcamp*, Udemy (online)
2022	*Complete Python Bootcamp from Zero to Hero in Python*, Udemy (online)
2020	*Build Websites from Scratch with HTML and CSS*, Udemy (online)
2018	*Theoretical Chemistry Summer School*, Center for Quantum Molecular Design, Stanford University, Stanford, California (USA)
2016	*VII National School of Photochemistry*, Department of Chemistry "G.Ciamician", University of Bologna, Bologna, Italy

Scientific Software Contributions

2021 **TeraChem Web Services**: web-based interface for quantum chemistry
2021 **MolAR**: iOS mobile application for visualizing molecules in augmeted reality
2020 **ChemVox**: Alexa skill for voice-controlled quantum chemistry

Awards

2021 **Wiley Outstanding Postdoc Award**, awarded by the American Chemical Society (COMP Division)
2021 **Best Flash Communication Award** at Sygenta Simposium 2021, awarded by the Swiss Chemical Society and Helvetica Chimica Acta
2017 **Guido Barone Award** for the best Ph.D thesis, awarded by the Italian Chemical Society (Campania Division)
2016 **Best Poster Communication Award** at IV National Meeting of the Theoretical and Computational Chemistry division of the Italian Chemical Society
2013 **Luigi Gomez Paloma Award** for the best master thesis, awarded by the Italian Chemical Society (Campania Division)

Teaching Experience

2017 **Instructor at the Gaussian Workshop**, Santiago De Compostela, Spain
2017 **Coordination Compound Chemistry** for master students in Chemical Sciences at the University of Naples Federico II – Assistance for lectures
2013-2018 **Computational Chemistry** for master students in Chemical Sciences at the University of Naples Federico II – Assistance for lectures and laboratory
2016-2018 **Topics in Physical Chemistry** for master students in Chemical Sciences at the University of Naples Federico II – Assistance for lectures and laboratory
2016-2018 **Chemical Physics** for bachelor students in Food science at the University of Naples Federico II – Assistance for lectures

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Mentoring of one PhD and three master students resulted in publications [5], [10], [15], [19].

Professional Services

Journal Reviewer

2018-present Mol. Catal., Theor. Chem. Acc., Phys. Chem. Chem. Phys., ChemistrySelect, Comput. Biol. Chem, J. Org. Chem., ACS Catal., J. Chem. Ed., RSC Advances

Meeting Organization

2020 Member of the organization committee of VCTC 2020
2018-2019 Italian Chemistry Olympiad for high school students
2016-2018 Open Day, Department of Chemical Sciences, University of Naples Federico II
2017 Staff member of the XXVI National Meeting of the Italian Chemical Society
2016 Staff member of the XLIV National meeting of the Physical Chemistry division of the Italian Chemical Society

Invited Seminar

2023 **Heinrich Heine University Düsseldorf**, Germany - Host: Prof. Jan Meisner
Molecular Dynamics Accelerated Reaction Discovery

2022 **University of Helsinki**, Finland - Host: Prof. Theo Kurten
Enhanced Sampling Aided Reaction Discovery

2018 **Stanford University**, CA, USA - Host: Prof. Todd Martinez
A Stairway to Heaven of Photoinduced Charge Transfer Reactions

2018 **KAUST University**, Saudi Arabia - Host: Prof. Luigi Cavallo
Modeling Artificial Leaf

Conference Contributions (selection)

28 contributions in national and international conference proceedings

2022 *Cutting-Edge Technologies in Computational Chemistry*, contributed poster at the **American Chemical Society Spring Meeting**

2020 *ChemVox: Voice-Controlled Quantum Chemistry*, contributed talk at the **2020 TeraChem Developers Meeting**

2017 *Ab Initio Molecular Dynamics to Simulate Excited State Proton Transfer to Solvent: The Strange Case of a Super Photoacid in Water and Methanol Solution*, contributed talk at the **XXVI National Meeting of the Italian Chemical Society**

2015 *Modeling of Proton Coupled Electron Transfer in the Framework of Density Functional Theory*, contributed talk at **Pacifichem**

Ab Initio Molecular Dynamics Combined with Different Solvation Models for Simulating Excited State Proton Transfer, contributed talk at **Pacifichem**

Publications

2023 **33**. Yang M., Raucci U., Parrinello M., *Reactant-Induced Dynamics of Lithium Imide Surfaces During the Ammonia Decomposition Process*, **Nat. Catal.**, 2023

32. Xu W., Sanchez D. M., Raucci U., Zhou H., Dong X., Hu M., Bardeen C. J., Martínez T. J., Hayward R. C., *Photo-Actuators via Epitaxial Growth of Microcrystal Arrays in Polymer Membranes*, **Nat. Mater.**, 2023, *22*, 1152

31. Das S., Raucci U., Neves R. P. P., Ramos M. J., Parrinello M., *How and When Does an Enzyme React? Unraveling -Amylase Catalytic Activity with Enhanced Sampling Techniques*, **ACS Catal.**, 2023, *13*, 8092

30. Raucci U., Weir H., Sakshuwong S., Seritan S., Hicks C., Vannucci F., Rea F., Martínez T. J., *Interactive Quantum Chemistry Enabled by Machine Learning, Graphical Processing Units, and Cloud Computing*, **Annu. Rev. Phys. Chem.**, 2023, *74*, 1

2022 **29**. Raucci U., Sanchez D. M., Martínez T. J., Parrinello M., *Enhanced Sampling Aided Design of Molecular Photoswitches*, **J. Am. Chem. Soc.**, 2022, *144*, 19265

28. Stricker F., Sanchez D. M., Raucci U., Dolinski N. D., Zayas M. S., Meisner J., Hawker C. J., Martínez T. J., Read de Alaniz J., *A Multi-Stage Single Photochrome System for Controlled Photoswitching Responses*, **Nat. Chem.**, 2022, *14*, 942

27. Raucci U., Weir H., Bannwarth C., Sanchez D. M., Martínez T.J., *Chiral Photochemistry of Achiral Molecules*, **Nat. Commun.**, 2022, *13*, 2091

26. Raucci U., Rizzi V., Parrinello M., *Discover, Sample, and Refine: Exploring Chemistry with Enhanced Sampling Techniques*, **J. Phys. Chem. Lett.**, 2022, *13*, 1424

25. Sakshuwong S., Weir H., Raucci U., Martínez T.J., *Bringing Chemical Structures to Life with Augmented Reality, Machine Learning, and Quantum Chemistry*, **J. Chem. Phys.**, 2022, *156*, 204801

2021

24. Sanchez D.M., Raucci U., Martínez T.J., *In Silico Discovery of Multistep Chemistry Initiated by a Conical Intersection: The Challenging Case of Donor–Acceptor Stenhouse Adducts*, **J. Am. Chem. Soc.**, 2021, *48*, 20015

23. Raucci U., Valentini A., Pieri E., Weir H.V., Seritan S., Martínez T.J. *Voice-Controlled Quantum Chemistry*, **Nat. Comput. Science**, 2021, *1*, 42

22. Chiariello M. G., Donati G., Raucci U., Perrela F., Rega N., *Structural Origin and Vibrational Fingerprints of the Ultrafast Excited State Proton Transfer of the Pyranine-Acetate Complex in Aqueous Solution*, **J. Phys. Chem. B**, 2021, *36*, 10273

21. Chiariello M. G., Raucci U., Donati G., Rega N., *Water Mediated Excited State Proton Transfer of Pyranine-Acetate in Aqueous Solution: Vibrational Fingerprints from Ab-Initio Molecular Dynamics*, **J. Phys. Chem. A**, 2021, *17*, 3569

20. Coppola F., Cimino P., Raucci U., Chiariello M. G., Petrone A., Rega N., *Exploring the Franck-Condon Region of a Photoexcited Charge Transfer Complex in Solution via Femtosecond Stimulated Raman Spectroscopy: Excited State Electronic Structure Methods to Unveil Non-Radiative Pathways*, **Chem. Sci.**, 2021, *12*, 8058

19. Tirri B., Mazzone G., Ottochian A., Gomar J., Raucci U., Adamo C., Ciofini., *A Combined Monte Carlo/DFT Approach to Simulate UV-vis Spectra of Molecules and Aggregates: Merocyanine Dyes as a Case Study*, **J. Comput. Chem.**, 2021, *42*, 1054

2020

18. Sanchez D.M., Raucci U., Ferreras K. N, Martínez T.J., *Putting Photomechanical Switches to Work: An Ab Initio Multiple Spawning Study of Donor–Acceptor Stenhouse Adducts*, **J. Phys. Chem. Lett.**, 2020, *11*, 7901

17. Raucci U., Savarese M., Adamo C., Ciofini I., Rega N., *Modeling the Electron Transfer Chain in an Artificial Photosynthetic Machine*, **J. Phys. Chem. Lett.**, 2020, *11*, 9738

16. Raucci U., Chiariello M. G., Rega N., *Modeling Excited State Proton Transfer to Solvent: a Dynamics Study of a Super-Photoacid with a Hybrid Implicit/Explicit Solvent Model*, **J. Chem. Theory and Comput.**, 2020, *16*, 7033

15. Raucci U., Perrella F., Donati G., Zoppi N., Petrone A., Rega N., *Ab-initio Molecular Dynamics and Hybrid Explicit-Implicit Solvation Model for Aqueous and non Aqueous Solvents: GFP Chromophore in Water and Methanol Solution as Case Study*, **J. Comput. Chem.**, 2020, *41*, 2228

14. Raucci U., Chiariello M. G., Coppola F., Perrella F., Savarese M., Ciofini I., Rega N., *An Electron Density Based Analysis to Establish the Electronic Adiabaticity of Proton Coupled Electron Transfer Reactions*, **J. Comput. Chem.**, 2020, *41*, 1835

13. Platella C., Raucci U., Rega N., D'Atri S., Levati L., Roviello G., Fuggetta M.P., Musumeci D., Montesarchio D., *Shedding Light on the Interaction of Polydatin and Resveratrol with G-Quadruplex and Duplex DNA: a Biophysical, Computational and Biological Approach*, **Int. J. Biol. Macromol.**, 2020, *151*, 1163

2019 **12**. Esposito R., Raucci U., Cucciolito M. E., Di Guida R., Scamardella C., Rega N., Ruffo F., *Iron(III) Complexes for Highly Efficient and Sustainable Ketalization of Glycerol: A Combined Experimental and Theoretical Study*, **ACS Omega**, 2019, *4*, 688

11. Chiariello M. G., Raucci U., Coppola F., Rega N. *Unveiling Anharmonic Coupling by Means of Excited State Ab Initio Dynamics: Application to Diarylethene Photoreactivity*, **Phys. Chem. Chem. Phys.**, 2019, *21*, 3606

2018 **10**. Perrella F., Raucci U., Chiariello M.G., Chino M., Maglio O., Lombardi A., Rega N., *Unveiling the Structure of a Novel Artificial Heme-Enzyme with Peroxidase-Like Activity: A Theoretical Investigation*, **Biopolymers**, 2018, *109*, e23225

9. Battista E., Scognamiglio P.L., Di Luise N., Raucci U., Donati G., Rega N., P.A. Netti, Causa F., *Turn-On Fluorescence Detection of Protein by Molecularly Imprinted Hydrogels Based on Supramolecular Assembly of Peptide Multi-Functional Blocks*, **J. Mater. Chem. B**, 2018, *6*, 1207

2017 **8**. Savarese M., Raucci U., Fukuda R., Adamo C., Ehara M., Rega N., Ciofini I., *Comparing the Performance of TD-DFT and SAC-CI Methods in the Description of Excited States Potential Energy Surfaces: an Excited State Proton Transfer Reaction as Case Study*, **J. Comput. Chem.**, 2017, *38*, 1084

2016 **7**. Raucci U., Ciofini I., Adamo C., Rega N., *Unveiling the Reactivity of a Synthetic Mimic of the Oxygen Evolving Complex*, **J. Phys. Chem. Lett.**, 2016, *7*, 5015

6. Savarese M., Raucci U., P.A. Netti, Adamo C., Rega N., Ciofini I., *A Qualitative Model to Identify Non-Radiative Decay Channels: the Spiropyran as Case Study*, **Theor. Chem. Acc.**, 2016, *135*, 211

5. Cimino P., Raucci U., Donati G., Chiariello M.G., Schiazza M., Coppola F., Rega N., *On the Different Strength of Photoacids*, **Theor. Chem. Acc.**, 2016, *135*, 117

2015 **4**. Raucci U., Savarese M., Adamo C., Ciofini I., Rega N., *Intrinsic and Dynamical Reaction Pathways of an Excited State Proton Transfer*, **J. Phys. Chem. B**, 2015, *119*, 2650

2014 **3**. Savarese M., Raucci U., Adamo C., Netti P.A., Ciofini I., Rega N., *Non Radiative Decay Paths in Rhodamines: New Theoretical Insights*, **Phys. Chem. Chem. Phys.**, 2014, *16*, 20681

2. Savarese M., Raucci U., Netti P.A., Adamo C.,Ciofini I., Rega N., *Modeling of Charge Transfer Processes to Understand Photophysical Singatures: The Case of Rhodamine 110*, **Chem. Phys. Lett.**, 2014, *610*, 148

1. Cusano A.M., Causa F., Della Moglie R., Falco N., Scogliamiglio P.L., Aliberti A., Vecchione R., Battista E., Marasco D., Savarese M., Raucci U., Rega N., Netti P.A., *Integration of Binding Peptide Selection and Multifunctional Particles as Tool-Box for Capture of Soluble Protein in Serum*, **J. R. Soc. Interface**, 2014, *11*, 20140718