Alessio Valentini Ph.D.

email: alevale@stanford.edu

Current position:

12/16/21-current | **Research Associate**, Stanford University, United States of America.

Education

02/16/20-12/15/21 | **Post Doc position**, Stanford University, United States of America. Post doc position on the project: *"Chemical reactivity with graph theory"*

11/01/16-01/31/2020 | **Post Doc position**, University of Liège, Belgium. FNRS Post doc on the project: *"Ultrafast photoinduced bond making"* and on the project: *"Exploiting Non-equilibrium Charge Dynamics in Polyatomic Molecules to Steer Chemical Reactions"*

10/01/15-08/31/16 | **Post Doc position**, University of Siena, Italy. Project title: *"Automatic Rhodopsin Modeling as a perspective Tool for High-Throughput Photobiology"*

11/12/11-09/30/15 | **Ph.D. in Computational Chemistry**, University of Alcalá, Spain. Thesis title: *"Semiclassical dynamics of natural and synthetic photoactive devices"*. Supervisor: Prof. Luis Manuel Frutos Gaite and Massimo Olivucci

10/08-04/11 | **M.Sc. in Chemistry for Sustainable Development**, University of Siena, Italy. Thesis title: *"Automatic generation of QM/MM models for photoactive proteins"*. Hosting lab: Bowling Green State University/University of Siena. Supervisor: Prof. Massimo Olivucci

10/03-04/07 | **B.Sc. in Chemistry**, University of Siena, Italy. Thesis title: *"Protein design using Rosetta"*. Hosting lab: Wageningen University and Research Centre. Supervisor: Prof. Jacques Vervoort

International conference oral communications

20/08/2018 | Valentini, A.; van den Wildenberg, S.; Remacle, F.; *"Photoinduced norbornadiene to quadricyclane isomerization using strong short femtosecond pulses."* - ACS meeting summer 2018, Boston, USA

20/08/2018 | Valentini, A.; Del Carmen Marín, M.; Agathangelou, D.; Orozco-Gonzalez Y.; Kandori, H.; Jung, K-H.; Haacke, S.; Olivucci M.; *"Towards the Computational Design of Highly Fluorescent Rhodopsins"* - ACS meeting summer 2018, Boston, USA

19/08/2018 | Valentini, A.; van den Wildenberg, S.; Remacle, F.; *"3-D electronic structure on the excited states manifold of Norbornadiene-Quadricyclane."* - ACS meeting summer 2018, Boston, USA

03/04/2018 | Valentini, A., *"Further development for semiclassical dynamics"* - Molcas Developers' Workshop 2018, Leuven, Belgium

22/07/2017 | Valentini, A., *"Towards the Computational Design of Highly Fluorescent Rhodopsins"* - ICP 2017, Strasbourg, France

30/03/2016 | Valentini, A., *"Report: semiclassical molecular dynamics"* - Molcas Developers' Workshop 2016, Siena, Italy

24/03/2014 | Valentini, A., Federico Melaccio, *"Photobiology and MOLCAS"* - Molcas Developers' Workshop 2014, Alcalá, Spain

29/01/2013	Valentini, A., *"New implementation in MOLCAS for nonadiabatic dynamics"* - Molcas Developers' Workshop 2013, Zurich, Switzerland

International conference written communications

07/29/2019	Valentini, A.; Aldaz, C.; Estrada, J.; Thompson, K.; Martínez, T.J.; *"High Throughput Chemistry"* - ACTC 2022, Lake Tahoe, California
07/29/2019	Valentini, A.; Aldaz, C.; Thompson, K.; Boswell, B.; Martínez, T.J.; *"Simulating reaction outcomes with graph theory"* - BATCHEM 2021, Virtual Conference.
07/29/2019	Valentini, A.; Thompson, K.; Woodward, A.; Punwong, C.; Martínez, T.J.; *"Learning Retrosynthesis Planning from ab initio data."* - VCTC 2020, Virtual Conference.
07/03/2019	Valentini, A.; van den Wildenberg, S.; Remacle, F.; *"Quantum dynamics of the isomerization of Norbornadiene to Quadricyclane induced by strong attopulses."* - ATTO 2019, Szeged, Hungary
08/19/2018	Valentini, A.; van den Wildenberg, S.; Remacle, F.; *"3-D electronic structure on the excited states manifold of Norbornadiene-Quadricyclane."* - ACS meeting summer 2018, Boston, USA. VIP sci-mix poster session
03/13/2018	Valentini, A.; van den Wildenberg, S.; Remacle, F.; *"3-D electronic structure on the excited states manifold of Norbornadiene-Quadricyclane."* - Jerusalem Nonadiabatica 2018, Jerusalem, Israel
06/28/2016	Valentini, A.; Manathunga M.; Yang X.; Luk H.; Gozem S.; Frutos L.M.; Ferré, N.; and Olivucci M. *"Probing the Photodynamics of Rhodopsins with Reduced Retinal Chromophores"* - The 8th Molecular Quantum Mechanics 2016, Uppsala, Sweden
09/16/2014	Valentini, A.; Gozem S.; Frutos L.M.; Olivucci M. *"Comparative dynamics of cis and trans isomerization in rhodopsins retinal models"* - 50th Symposium on Theoretical Chemistry 2014, Vienna, Austria
07/16/2012	Valentini, A.; Marazzi, M.; Melaccio, F.; Gozem, S.; Olivucci, M.; Frutos, L.M. *"Local CASPT2/CASSCF gradient scaling on QM and QM/MM rhodopsin models"* - 24th IUPAC Symposium on Photochemistry, Coimbra, Portugal

Computer skills and competences

O.S.	CentOS, Ubuntu, Windows
Prog. Languages	Python, Haskell, Cython
Graphics	Gimp, Blender, Inkscape
Misc. Programs	LaTeX, JupyterLab, Docker

Software development projects

OpenMolcas	Multiconfigurational post-Hartree-Fock Electronic Structure Calculations. Developer for module DYNAMIX and SURFACEHOP
HsDynamics	Semi-Classical Molecular Dynamics in Haskell. Mentioned into HCAR 2013
HsFock	Ab-initio electronic structure in Haskell. Mentioned into HCAR 2013
DynAnalyzer	A collection of Haskell Tools to analyze bulks of M.D. trajectories
GridQuantum	A program that propagates nuclear quantum wavepackets into electronic PES on a grid
pydensity	A tool for the calculation and visualization of electronic densities in multidimensional wavefunctions

InteraChem	Iteractive Molecular dynamics in virtual reality
ChemVox	ChemVox performs real-time quantum chemistry calculations from a voice command and returns the results in seconds
Retropath	A tool for exploiting graph matching and *ab-initio* calculations to plan any molecule syntheses

Awards

- BATCHEM 2021 first prize for best lightning talk.
- ACS 2018 - Poster selected for VIP sci-mix posters.

Publications submitted or in preparation

- Valentini, A.; Aldaz, C.; Thompson, K.; Boswell, B.; Martínez,T.J.; *"Retropaths – a retrosynthesis program for discovering new chemistry"*, in preparation.

Publications

21. Wang, Y.; Seritan, S.; Lahana, D.; Ford, Jason; Valentini, A.; Hohenstein, E.; Martínez, T.J.; *"InteraChem: Exploring Excited States in Virtual Reality with Ab Initio Interactive Molecular Dynamics"*, J. Chem. Theory Comput., **2022**, *18* (16), 3308–3317, **DOI:** 10.1021/acs.jctc.2c00005

20. Seritan, S.; Wang, Y.; Ford, J.E.; Valentini, A.; Gold, T; Martínez,T.J.; *"InteraChem: Virtual Reality Visualizer for Reactive Interactive Molecular Dynamics"*, J. Chem. Educ., **2021**, *98* (11), 3486–3492, **DOI:** 10.1021/acs.jchemed.1c00654

19. Raucci, U.; Valentini, A.; Pieri, E.; Weir, H.; Seritan, S.; Martínez,T.J.; *"Voice-Controlled Quantum Chemistry"*, Nat. Comput. Sci., **2021**, *1*, 42–45 **DOI:** 10.1038/s43588-020-00012-9

18. Valentini, A.; van den Wildenberg, S.; Remacle, F.; *"Selective bond formation triggered by short optical pulses: quantum dynamics of a four-center ring closure"*, Phys. Chem. Chem. Phys., **2020**, *22*, 22302-22313, **DOI:** 10.1039/D0CP03435E

17. Aquilante, F.; Autschbach, J.; Baiardi, A.; Battaglia, S.; Borin, V.A.; Chibotaru, L.F.; Conti, I.; De Vico, L.; Delcey, M.; Fdez. Galván, I.; Ferré, N.; Freitag, L.; Garavelli, M.; Gong, X.; Knecht, S.; Larsson, E.D.; Lind, R.; Lundberg, M.; Malmqvist, P.Å.; Nenov, A.; Norell, J.; Odelius, M.; Olivucci, M.; Pedersen, T.B.; Pedraza-González, L.; Quan M. Phung, Pierloot, K.; Reiher, M.; Schapiro, I.; Segarra-Martí, J.; Segatta, F.; Seijo, L.; Sen, S.; Sergentu, D.; Stein, C.J.; Ungur, L.; Vacher, M.; Valentini, A.; Veryazov, V.; *Modern quantum chemistry with [Open]Molcas"*, J. Chem. Phys., **2020**, *152* (214117), **DOI:** 10.1063/5.0004835

16. Pedraza-González, L.; del Carmen Marín M.; Jorge, A.; D. Ruck, T.; Yang, X.; Valentini, A.; Olivucci, M.; De Vico, L.; *"Web-ARM: a Web-Based Interface for the Automatic Construction of QM/MM Models of Rhodopsins"*, J. Chem. Inf. Model., **2020**, *60* (3), 1481–1493, **DOI:** 10.1021/acs.jcim.9b00615

15. Fdez. Galván, I.; Vacher, M.; Alavi, A.; Angeli, C.; Aquilante, F.; Autschbach, J.; J. Bao, J.; I. Bokarev, S.; A. Bogdanov, N.; K. Carlson, R.; F. Chibotaru, L.; Creutzberg, J.; Dattani, N.; G. Delcey, M.; Dong, S.; Dreuw, A.; Freitag, L.; Manuel Frutos, L.; Gagliardi, L.; Gendron, F.; Giussani, A.; Gonzalez, L.; Grell, G.; Guo, M.; E. Hoyer, C.; Johansson, M.; Keller, S.; Knecht, S.; Kovačević, G.; Källman, E.; Li Manni, G.; Lundberg, M.; Ma, Y.; Mai, S.; Pedro Malhado, J.; Åke Malmqvist, P.; Marquetand, P.; A. Mewes, S.; Norell, J.; Olivucci, M.; Oppel, M.; Manh Phung, Q.; Pierloot, K.; Plasser, F.; Reiher, M.; M. Sand, A.; Schapiro, I.; Sharma, P.; J. Stein, C.; Kragh Sørensen, L.; G. Truhlar, D.; Ugandi, M.; Ungur, L.; Valentini, A.; Vancoillie, S.; Veryazov, V.; Weser, O.; Wesolowski, T. A.; Widmark, P.; Wouters, S.; Zech, A.; Patrick Zobel, J.; Lind, R.; *"OpenMolcas: From Source Code to Insight"*, J. Chem. Theory Comput., **2019**, *15*, 11, 5925-5964 **DOI:** 10.1021/acs.jctc.9b00532

14. Valentini, A.; Nucci, M.; Frutos, L. M.; Marazzi, M. *"Photosensitized Retinal Isomerization in Rhodopsin Mediated by a Triplet State"*, ChemPhotoChem, **2019**, **DOI:** 10.1002/cptc.201900067R1

13. del Carmen Marín M.; Gathangelou, D.; Orozco-Gonzalez, Y.; Valentini, A.; Kato, Y.; Abe-Yoshizumi, R.; Kandori, H.; Choi, A.; Jung, K-H.; Haacke, S.; Olivucci, M. *"Fluorescence enhancement of a microbial rhodopsin via electronic reprogramming"*, J. Am. Chem. Soc., **2019**, *141* (1), 262–271, **DOI:** 10.1021/jacs.8b09311

12. Schnedermann C.; Yang X.; Liebel M.; Spillane K. M.; Lugtenburg J.; Fernandez I.; Valentini, A.; Shapiro I.; Olivucci M.; Kukura P.; Mathies R. A. *"Evidence for a vibrational phase isotope effect on the photochemistry of vision"*, Nature Chemistry, **2018**, *10* 4, 449-455, **DOI:** 10.1038/s41557-018-0014-y

11. Vacher M.; Farahani P.; Valentini, A.; Karlsson H. O.; Galván, I.; Frutos, L. M.; Lindh R. *"Unraveling the chemiluminescence yield of 1,2-dioxetanes"*, J. Phys. Chem. Lett., **2017**, *8*, 3790–3794, **DOI:** 10.1021/acs.jpclett.7b01668

10. Valentini, A.; Rivero, D.; Zapata, F.; García-Iriepa, C.; Marazzi, M.; Palmeiro, R.; Galván, I.; Sampedro, D.; Olivucci, M.; Frutos, L. M. *"Optomechanical control of quantum yield in trans-cis ultrafast photoisomerization of a retinal chromophore model"*, Angewandte Chemie, **2017**, *56* (14), 3842-3846, **DOI:** 10.1002/anie.201611265

9. Melaccio, F.; del Carmen Marín M.; Valentini, A.; Montisci, F.; Rinaldi, S.; Cherubini, M.; Kato Y.; Stenrup M.; Orozco-Gonzalez Y.; Ferré, N.; Luk H.; Kandori H.; Olivucci, M. *"Towards Automatic Rhodopsin Modeling as a Tool for High-throughput Computational Photobiology"*, J. Chem. Theory Comput., **2016**, *12* (12), 6020–6034, **DOI:** 10.1021/acs.jctc.6b00367

8. Melaccio, F.; Calimet, N.; Schapiro, I.; Valentini, A.; Cecchini, M.; Olivucci, M. *"Space and Time Evolution of the Electrostatic Potential During the Activation of a Visual Pigment"*, J. Phys. Chem. Lett., **2016**, *7*(13), 2563–2567, **DOI:** 10.1021/acs.jpclett.6b00977

7. Aquilante, F.; Autschbach, J,; Carlson, R. K.; Chibotaru, L. F.; Delcey, M. G.; De Vico, L.; Galván, I.; Ferré, N.; Frutos, L. M.; Gagliardi, L.; Garavelli, M.; Giussani, A.; Hoyer, C. E.; Li Manni, G.; Lischka, H.; Ma, D.; Malmqvist, P.Å.; Müller, T.; Nenov, A.; Olivucci, M.; Pedersen, T. B.; Peng, D.; Plasser, F.; Pritchard, B.; Reiher, M.; Rivalta, I.; Schapiro, I.; Segarra-Martí, J.; Stenrup, M.; Truhlar, D. G.; Ungur, L.; Valentini, A.; Vancoillie, S.; Veryazov, V.; Vysotskiy, V.P.; Weingart, O.; Zapata, F.; Lindh R. *"Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table "*, J. of Comput. Chem., **2016**, *37*, 506–541, **DOI:** 10.1002/jcc.24221

6. Manathunga, M.; Yang, X.; Luk, H.; Gozem, S.; Valentini, A.; Frutos, L. M.; Ferré, N.; Olivucci, M. *"Probing the Photodynamics of Anabaena Sensory Rhodopsin with Reduced Retinal Chromophores"*, J. Chem. Theory Comput., **2015**, *12*(2), 839-850, **DOI:** 10.1021/acs.jctc.5b00945

5. Rivero, D.; Valentini, A.; Fernández-González, M. A.; García-Iriepa, C.; Sampedro, D.; Palmeiro, R.; Frutos, L. M. *"Mechanical Forces Alter Conical Intersections Topology"*, J. Chem. Theory Comput., **2015**, *11*, 3740–3745, **DOI:** 10.1021/acs.jctc.5b00375

4. Marchand, G.; Eng, J.; Schapiro, I.; Valentini, A.; Frutos L.M.; Pieri, E.; Olivucci, M.; Léonard J.; Gindensperger, E. *"Directionality of Double Bond Photoisomerization Dynamics Induced by a Single Stereogenic Center"*, J. Phys. Chem. Lett., **2015**, *6*, 599-604, **DOI:** 10.1021/jz502644h

3. Gozem, S.; Melaccio, F.; Valentini, A.; Filatov, M.; Huix-Rotllant, M.; Ferré, N.; Frutos L.M. ; Angeli, C.; Krylov, A.; Granovsky, A.; Lindh, R.; Olivucci, M. *"On the Shape of Multireference, EOM-CC, and DFT Potential Energy Surfaces at a Conical Intersection"*, J. Chem. Theory Comput., **2014**, *10* (8), 3074–3084, **DOI:** 10.1021/ct500154k

2. García-Iriepa, C.; Marazzi, M.; Zapata, F.; Valentini, A.; Sampedro, D.; Frutos L.M. *"Chiral Hydrogen Bond Environment Providing Unidirectional Rotation in Photoactive Molecular Motors"*, J. Phys. Chem. Lett., **2013**, *4* (9), 1389-1396, **DOI:** 10.1021/jz302152v

1. Laricheva, E.N.; Gozem, S.; Rinaldi, S.; Melaccio, F.; Valentini, A.; Olivucci, M. *"Origin of fluorescence in 11-cis locked bovine rhodopsin"*, J. Chem. Theory Comput., **2012**, *8* (8), 2559-2563, **DOI:** 10.1021/ct3002514

Languages

Italian	Mother tongue
English	Fluent in speech, writing and reading
Spanish	Fluent in speech and reading. Basic in writing
French	Basic in speech, writing and reading