Alessio Valentini Ph.D.

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Current position:

02/16/20-current	**Post Doc position**, Stanford University, United States of America. Post doc position on the project: *"ab initio interactive molecular dynamics"*

Education

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.; Thompson, K.; Woodward, A.; Punwong, C.; Martínez,T.J.; *"Learning Retrosynthesis Planning from ab initio data."* - VCTC 2020, Virtual Conference.
07/29/2019	Wang, Y.; Seritan, S.; Valentini, A.; Ford, J.E.; Martínez,T.J.;*"Ab Initio Interactive Molecular Dynamics: A Hands-On Experience with Quantum Chemistry"* - 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	Manathunga M.; Yang X.; Luk H.; Gozem S.; Frutos L.M.; Valentini, A.; 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
07/16/2012	García-Iriepa C.; Marazzi, M.; Zapata, F.; Valentini, A.; Castaño, O.; Sampedro, D.; Frutos, L.M.*"Hydrogen bonds in molecular motors as a way to achieve unidirectional rotation: a mechanistic and dynamical study."* - 24th IUPAC Symposium on Photochemistry, Coimbra, Portugal

Computer skills and competences

O.S.	CentOS, Ubuntu, OpenSuse, Windows
Prog. Languages	Haskell, Python, Cython, Bash, Fortran
Scientific Software	OpenMolcas, Tinker, VMD
HPC	Ansible, Easybuild, LDAP, Torque/Maui, Slurm
Graphics	Gimp, Blender, Inkscape
Misc. Programs	LaTeX, ViM, Git, 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

Publications submitted or in preparation

- Valentini, A.; van den Wildenberg, S.; Remacle, F.; *"Quantum dynamics of the isomerization of Norbornadiene to Quadricyclane induced by strong attopulses."*, submitted to Physical Chemistry Chemical Physics.
- Seritan, S.; Wang, Y.; Ford, J.E.; Valentini, A.; Gold, T; Martínez,T.J.; *"InteraChem: A Visualizer for Reactive Interactive Molecular Dynamics in Virtual Reality"*, in preparation.
- Raucci, U.; Valentini, A.; Pieri, E.; Weir, H.; Seritan, S.; Martínez,T.J.; *"ChemVox: Voice-Controlled Quantum Chemistry"*, in preparation.
- Thompson, K.; Valentini, A.; Punwong, C.; Woodward, A.; Martínez,T.J.; *"Retropaths – a retrosynthesis program for discovering new chemistry"*, in preparation.

Publications

- 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
- 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
- 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
- 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
- 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
- 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
- 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

- 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

- 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

- 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

- 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

- 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

- 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

- 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

- 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

- 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

- 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