Curriculum Vitae

Basile F. E. Curchod

Department of Chemistry
Durham University, UK
☎ +44 (0)1913 34 40 65
✉ basile.f.curchod@durham.ac.uk
www.in-silico-photochem.com
Swiss citizen, 33 years old

Last updated: February 11, 2018

Academic Appointments

Present

11/2017 – Present **Assistant Professor in Theoretical Chemistry**, *Department of Chemistry, Durham University*, UK.
In Silico Photochemistry Group

Past

05/2016 – 10/2017 **Marie Skłodowska-Curie Research Fellow**, *School of Chemistry, University of Bristol*, UK.
Centre for Computational Chemistry.

12/2015 – 05/2016 **Postdoctoral Researcher**, *Theory Department, Max-Planck Institute of Microstructure Physics, Halle*, Germany.
Advisor: Prof. Eberhard K. U. Gross.

05/2014 – 11/2015 **Postdoctoral Scholar**, *Department of Chemistry, Stanford University, Stanford*, USA.
Advisor: Prof. Todd J. Martínez.

01/2014 – 04/2014 **Invited Researcher**, *Laboratory for Computational Molecular Design, EPFL*, Lausanne, Switzerland.
Advisor: Prof. Clémence Corminboeuf.

Education

05/2009 – 09/2013 **Ph.D. in Theoretical Chemistry**, *Laboratory of Computational Chemistry and Biochemistry, EPFL*, Lausanne, Switzerland.
Title: "A Classical and Quantum Trajectory Description of Nonadiabatic Dynamics using Time-Dependent Density Functional Theory", Dr. MER Ivano Tavernelli (supervisor) and Prof. Ursula Röthlisberger (advisor). Selected for the PhD Research Award 2013.

09/2007 – 04/2009 **M.Sc. in Chemistry**, *EPFL*, Lausanne, Switzerland.
Orientation: Theoretical and Physical Chemistry.
Master Thesis: "Towards the Binding of Cisplatin to Cu,Zn Superoxide Dismutase: First Steps of a Theoretical Study", Laboratory of Computational Chemistry and Biochemistry.

09/2004 – 08/2007 **B.Sc. in Chemistry and Chemical Engineering**, *EPFL*, Lausanne, Switzerland.

Publications

49 peer-reviewed articles spanning the fields of chemistry and physics, 1 book on general chemistry, 1 book chapter, and 1 popular science article. Total of 3759 citations, h-index of 22 (Google Scholar, February 2018), including publications in high-profile journals, *e.g.* Nature Chemistry and Angewandte Chemie International Edition.

Research Grants

06/2016 **COST Short-Time Scientific Mission (STSM)**, *Project "Conical intersection – a mirage within the exact factorization of the molecular wavefunction?" – €1,500 (£1,300)*, COST Action MP1306 EUSpec.

01/2016 **Marie Skłodowska-Curie Individual Fellowship**, *Project "NonAdiabatic Molecular Dynamics of organic Intermediates in Atmospheric chemistry" (NAMDIA) – €183,000 (£157,000) over 2 years*, European Commission Research & Innovation.

11/2013 **Early Postdoc.Mobility Grant**, *Project "Ab initio Multiple Spawning and GPU-based Excited Electronic State Dynamics for the Realistic Simulation of Nonadiabatic Phenomena in Energy-related Devices" – CHF90,000 (£77,000) over 1.5 year*, Swiss National Science Foundation.

Selected Awards

03/2015 **MCC Travel Award**, *NSF grant, Materials Computation Center, University of Illinois Urbana-Champaign*.

11/2013 **Teaching Excellency Award**, *Section of Chemistry, EPFL*.

09/2012 **Best Oral Presentation in Computational Chemistry**, *Swiss Chemical Society*.

09/2011 **Best Oral Presentation in Computational Chemistry**, *Swiss Chemical Society*.

05/2011 **Chemistry Travel Award**, *Swiss Academy of Science/Swiss Chemical Society*.

07/2010 **Best Poster**, *CCP6 Workshop on Quantum Trajectories, Bangor University*.

11/2009 **Selected as "Young Researcher"**, *59th Meeting of Nobel Laureates, Lindau*.

10/2009 **Prize "CIBA SA"**, *Best Master Thesis, EPFL*.

10/2008 **Prize "Syngenta Monthey"**, *Best Average Grade (Master), EPFL*.

10/2007 **Prize "Pelet"**, *Best Average Grade (Bachelor), EPFL*.

03/2007 **Excellency Scholarship**, *EPFL*.

Teaching Experience

Lecturer

Since 01/2018 **"Applied Quantum Mechanics"**, *Advanced Computational Chemistry Module*, Durham University (UK).

Since 11/2017 **"Quantum Mechanics"**, *Computational Chemistry Module*, Durham University (UK).

Invited Lecturer

17/05 – 18/05 2018 **"Ab initio nonadiabatic molecular dynamics"**, *4 hrs, CECAM School "Quantum and Mixed Quantum Classical Dynamics in photochemistry"*, Zaragoza (Spain).

20/01/2017 **"Ab Initio Nonadiabatic Molecular Dynamics"**, *2 hrs, Virtual Winter school of Computational Chemistry*, University of Bristol (UK).

07/10/2016 **"Nonadiabatic Molecular Dynamics with Ab Initio Multiple Spawning"**, *2 hrs, Workshop on Surface Hopping*, University of Vienna (Austria).

02/08/2016 **"Ab Initio Multiple Spawning with TeraChem"**, *2 hrs, Theory Tutorials*, SLAC, Menlo Park (USA).

07/03 – 14/03 2014 **"Computational Chemistry for High-School Students"**, *2 hrs, Chemistry Days*, EPFL, Lausanne (Switzerland).

08/04 – 12/04 2013 **"Ab initio nonadiabatic molecular dynamics"**, *4 hrs, School on Molecular Excited States, European Master on Theoretical Chemistry and Computational Modelling*, Zaragoza (Spain).

04/06 – 08/06 2012 **"TDDFT for ultrafast electronic dynamics"**, *4 hrs, School on Molecular Excited States, European Master on Theoretical Chemistry and Computational Modelling*, Zaragoza (Spain).

10/05 – 12/05 2012 **"Nonadiabatic Dynamics"**, *2 hrs, CECAM tutorial: Nonadiabatic Quantum Dynamics*, Lausanne (Switzerland).

30/05 – 03/06 2011 **"TDDFT for ultrafast electronic dynamics"**, *6 hrs, European School on the dynamics of molecular excited states*, Zaragoza (Spain).

02/01 – 15/01 2010 **"TDDFT as a tool for Chemistry and Biochemistry"**, *2 hrs, Winter School on TDDFT: Prospects and Applications*, Benasque (Spain).

Supervisor and Teaching Assistant

2017-Present **Demonstrator**, *Workshops and Practicals, "Quantum Mechanics"*, Durham University (UK).

2015-Present **Advisor**, *4 PhD students, different projects related to nonadiabatic dynamics*, EPFL (Switzerland), Stanford University (USA), and Bristol (UK).

2016-2017 **Demonstrator**, *Computational class on Molecular Orbitals*, University of Bristol (UK).

2017 **Supervisor**, *1 advanced student project*, EPSRC Centre for Doctoral Training in Theory and Modelling in Chemical Sciences, Bristol (UK).

2013-2014 **Co-supervisor**, *Master thesis project, "Analytical gradients in FOMO-CASSCI"*, EPFL (Switzerland) and Stanford University (USA).

2012-2013 **Supervisor**, *Master thesis project, "Spin-orbit coupling within LR-TDDFT"*, EPFL (Switzerland).

2011-2013 **Supervisor**, *2 different semester projects for Master students*, EPFL (Switzerland).

2010-2013 **Supervisor**, *4 different semester projects for the Bachelor course entitled "Introduction to electronic structure methods"*, EPFL (Switzerland).

2009-2013 **First assistant**, *Master lecture: "Computational methods in molecular quantum mechanics"*, EPFL (Switzerland).

2009-2013 **First assistant and co-organizer**, *Practical works for first-year Bachelor students on "Computers in Chemistry"*, EPFL (Switzerland).

2010-2011 **First assistant**, *Master lecture: "Applied molecular quantum chemistry"*, EPFL (Switzerland).

Others

2016-Present **Virtual Reality to Teach Chemistry**, *Demonstration and presentation of interactive Virtual Reality, produced by interactive Scientific, Bristol*, UK.

2008-2012 **Scientific writer**, *Co-author of the general chemistry book entitled "Introduction à la Chimie"*, LEP Editions, Lausanne (Switzerland).

2010-2013 **PhD student delegate**, *Teaching commission for Chemistry*, EPFL (Switzerland).

Scientific Presentations

Invited Talks

07/06/2018 **Thomas Young Centre Soiree "Excited states dynamics"**, *London (UK)*.

16/04/2018 **AMOC2018**, *Budapest (Hungary)*.

29/03/2018 **FMS/TeraChem Developer's Meeting**, *Stanford (USA)*.

14/02/2018 **Condensed Matter Physics Seminar**, *Durham University (UK)*.

15/01/2018 **Chemistry and Mathematics in Phase Space Meeting**, *Bristol (UK)*.

08/01/2018 **Theoretical and Experimental Photochemistry at VUV-X Energy Ranges, COST Meeting**, *Bristol (UK)*.

15/08/2017 **Physikalisches Kolloquium**, *Max Planck Institute for Polymer Research, Mainz (Germany)*.

21/07/2017 **28th International Conference on Photochemistry**, *Strasbourg (France)*.

13/07/2017 **PULSE Seminar, SLAC**, *Menlo Park (USA)*.

25/05/2017 **Massive Computation for Ultrafast Molecular Breaking (MACUMB 2017)**, *Madrid (Spain)*.

03/03/2017 **Theoretical Chemistry Seminar**, *University of Chemistry and Technology Prague (Czech Republic)*.

28/02/2017 **Physical Chemistry Seminar**, *Université de Genève (Switzerland)*.

15/12/2016 **Chemistry Seminar**, *Université de Liège (Belgium)*.

13/12/2016 **Computational Chemistry Seminar**, *University of Bristol (UK)*.

30/11/2016 **Department Seminar**, *University of Leeds (UK)*.

03/11/2016 **Physical Chemistry Seminar**, *Université Paris-Sud (France)*.

20/05/2016 **School of Chemistry Seminar**, *University of Birmingham (UK)*.

13/05/2016 **Atmospheric Chemistry Seminar**, *University of Leeds (UK)*.

18/03/2016 **Physical Chemistry Seminar**, *University of Jena (Germany)*.

22/01/2016 **14th Swiss Snow Symposium 2016, Swiss Young Chemists' Association**, *Saas Fee (Switzerland)*.

27/11/2015 **Chemical Dynamics and Molecular Spectroscopy Seminar**, *University of Bristol (UK)*.

19/11/2015 **Physical Chemistry Symposium**, *University of Basel (Switzerland)*.

11/11/2015 **Theory Department Seminar**, *University of Vienna (Austria)*.

29/09/2014 **Physics Salon of Palo Alto**, *Palo Alto (USA)*.

23/03/2012 **4th Annual Meeting of the COST Action CUSPFEL**, *Cluj (Romania)*.

Contributed Talks

28/08/2017 **11th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC)**, *Munich (Germany)*.

06/06/2017 **Seeking synergy between dynamics and statistics for non-equilibrium quantum processes, CECAM Workshop**, *Paris (France)*.

19/03/2017 **Computational Molecular Science 2017**, *Warwick (UK)*.

08/11/2016 **Excited State Simulations: Bridging Scales**, *Marseille (France)*.

14/09/2016 **MOLEC 2016, European Conference on the Dynamics of Molecular Systems**, *Toledo (Spain)*.

05/03/2015 **American Physical Society, March Meeting**, *San Antonio (USA)*.

06/09/2013 **Swiss Chemical Society, Fall meeting**, *Lausanne (Switzerland)*.

09/01/2013 **NCCR MUST Annual Meeting**, *Engelberg (Switzerland)*.

13/09/2012 **Swiss Chemical Society, Fall meeting**, *Zurich (Switzerland)*.

09/09/2011 **Swiss Chemical Society, Fall meeting**, *Lausanne (Switzerland)*.

18/07/2011 **Ninth Triennal Congress of the WATOC**, *Santiago de Compostela (Spain)*.

03/11/2010 **Adiabatic and Nonadiabatic Methods in Quantum Dynamics, CECAM Workshop**, *Lausanne (Switzerland)*.

Science Outreach

2017 – Present **Animation of the workshop "Micro-Choregraphy", dynamics of the microscopic world using virtual reality**, *Different festivals and conferences like: Transmediale Digital Culture Festival 2017, Berlin (Germany) & VR World Congress, Bristol (UK)*.

05/2016 **Co-editor**, *Special issue of the Interalia Magazine, on the topic "Micro-Choregraphy", interactions between the arts, sciences and consciousness.*.

Posters

19/09/2016 **Reaction Rate Theory: Faraday Discussion**, *Cambridge (UK)*.

16/06/2015 **Molecular Quantum Dynamics Methods: Benchmarks and State of the Art, CECAM Workshop**, *Lausanne (Switzerland)*.

2/06/2012 **18th International Conference on Ultrafast Phenomena**, *Lausanne (Switzerland)*.

12/04/2012 **High-dimensional Quantum Dynamics, CECAM Workshop**, *Birmingham (UK)*.

15/02/2012 **Swiss Association of Computational Chemists, Annual Meeting**, *Bern (Switzerland)*.

08/01/2012 **NCCR MUST Annual Meeting**, *Lenk (Switzerland)*.

25/09/2011 **European School in Quantum Chemistry**, *Palermo (Italy)*.

16/09/2010 **Swiss Chemical Society, Fall meeting**, *Zurich (Switzerland)*.

14/07/2010 **CCP6 Workshop on Quantum Trajectories**, *Bangor, Wales (UK)*.

Conference and School Organization

09/07 – 20/07 2018 **E-CAM Extended Software Development Workshop**, *ESDW10: Quantum Dynamics*, Paris (France), co-organizer.

26/02 – 02/03 2018 **CECAM School**, *Nonadiabatic Molecular Dynamics in Three Different Flavors*, Lausanne (Switzerland), co-organizer.

10/01 – 12/01 2018 **COST Meeting**, *WG3, UV and X-ray photochemistry – COST action "Our Astro-Chemical History"*, Bristol (UK), co-organizer.

31/03/2017 **Mini-Symposium**, *Excited-State Dynamics with Travelling Gaussians*, Bristol (UK), Organizer.

06/06 – 10/06 2016 **CECAM Workshop**, *Different Routes to Quantum Molecular Dynamics*, Lausanne (Switzerland), co-organizer.

12/05 – 15/05 2014 **CECAM Workshop**, *Recent Progress in Adiabatic and Nonadiabatic Methods in Quantum Dynamics*, Lausanne (Switzerland), co-organizer.

10/05 – 12/05 2012 **CECAM Tutorial**, *Nonadiabatic Quantum Dynamics with MCTDH and CPMD*, Lausanne (Switzerland), co-organizer.

01/11 – 03/11 2010 **CECAM Workshop**, *Adiabatic and Nonadiabatic Methods in Quantum Dynamics*, Lausanne (Switzerland), co-organizer.

Additional Academic Activities and Experience

02/2018 – Present **Member of the Editorial Board for the Journal "Molecules", published by MDPI**.

02/2018 – Present **Organizer of the Departmental Seminars**, *Durham University*, UK.

02/2018 – Present **Member of the HPC Steering committee**, *Durham University*, UK.

01/2018 – Present **Ordinary Member, Committee of the "Spectroscopy and Dynamics Group"**, *Royal Society of Chemistry*, UK.

11/2017 – Present **Invited Researcher**, *School of Chemistry, University of Bristol*, UK.

11/2016 – Present **Member of the Royal Society of Chemistry**.

2014 – Present **Active referee for the following journals**, *J. Phys. Chem. Lett., J. Chem. Phys., Phys. Chem. Chem. Phys., J. Chem. Theory Comput., ChemPhysChem, Int. J. Quantum Chem., RSC Adv., Dalton Trans., J. Lumin., Chem. Select, and ChemSusChem*.

01/2017 – 10/2017 **Organizer of the "Computational Chemistry Seminars"**, *School of Chemistry*, University of Bristol, UK.

11/2015 **Invited Royal Society Researcher**, *Host: FRSC Dr. David R. Glowacki*, University of Bristol, UK.

08/2008 **Visiting Student**, *Organometallic chemistry*, Imperial College, London (UK).

07/2007 **Trainee in Phytochemistry**, *Laboratoire de Pharmacognosie et de Phytochimie*, University of Geneva (Switzerland).

07/2006 **Trainee in Quality Control Lab**, *SEROLAB SA*, Remaufens (Switzerland).

National and International Collaborators

- **Dr. Federica Agostini**, Laboratoire Chimie Physique, Université Paris-Sud (France). *Exact factorization for nonadiabatic dynamics (theory).*
- **Dr. Thomas J. Penfold**, School of Chemistry, University of Newcastle (UK). *Nonadiabatic dynamics of metal complexes (theory).*
- **Dr. Benoît Mignolet**, Department of Chemistry, Université de Liège (Belgium). *Electron dynamics in molecules (theory).*
- **Dr. Ivano Tavernelli**, IBM Research Center (Switzerland). *Ehrenfest and trajectory surface hopping dynamics (theory).*
- **Prof. Michael N. R. Ashfold**, **Prof. Andrew J. Orr-Ewing**, and **Dr. Tom A. A. Oliver**, University of Bristol (UK). *Ultrafast spectroscopy of molecules in gas phase and solution (experiment).*
- **Prof. Todd J. Martínez**, Stanford University (USA). *Nonadiabatic dynamics (theory).*

Languages

French **Native speaker**

English **Proficient user**

German **Independent user**