Maximilian A. C. Saller

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Date of Birth: 5/1/1991 • Citizenship: German • Visa Status: Green Card Holder

Education and Employment

Kent State University, Kent, OH, USA
Postdoctoral Research Fellow *2022–present*
Working in the group of Prof. Barry Dunietz, focusing on developing and applying screened range separated hybrid functionals within density functional theory to energy and charge transfer in biologically interesting systems.

University of Michigan, Ann Arbor, MI, USA
Visiting Scholar *2022–present*
Continuing work in the group of Prof. Eitan Geva. Focusing on calculating cavity modified rates of reaction using cavity-free inputs to allow for computationally guided design of experiments. Work has been published in international journals (*The Journal of Physical Chemistry C*).

Postdoctoral Research Fellow *2020–2022*
Working in the group of Prof. Eitan Geva in the Department of Chemistry. Continued development of the improved mapping method and demonstrated its applicability and effectiveness for cavity modified molecular quantum dynamics. Work has been published in international journals (*The Journal of Physical Chemistry Letters*) and presented at national conferences.

Swiss Federal Institute of Technology (ETH Zurich), Zurich, Switzerland
ETH Postdoctoral Fellow *2018–2020*
Competitive 24-month postdoctoral fellowship financed through the European Commission (valued at $250,000). Awarded based on a grant application including a detailed research proposal and interview panel. Continuing the project with Prof. Jeremy Richardson.

Postdoctoral Researcher *2017–2018*
Extending non-adiabatic ring polymer molecular dynamics: Long-time quantum dynamics from short-time trajectories.
Working in the group of Prof. Jeremy Richardson. Developed an improved semiclassical mapping approach for simulation of nonadiabatic quantum dynamics which has drastically improved the performance of mapping methods for population based observables in a variety of systems. Work has been published in international journals (*The Journal of Chemical Physics*, *Faraday Discussions*), in book chapter form and presented at national and international conferences.

University of Warwick, Coventry, United Kingdom
PhD in Theoretical Chemistry *2013–2017*
Sampling minimal, adaptive basis sets for multidimensional, nuclear quantum dynamics using simple, semi-classical trajectories.
Working in the group of Prof. Scott Habershon. Developing a new hybrid quantum dynamics method relying on semiclassical trajectories to sample phase space and generate a static quantum basis set which is then used to propagate dynamics using variational equations of motion. This approach addresses the curse of dimensionality which commonly limits wavefunction based quantum dynamics methods. Extending this approach using a matching pursuit algorithm to optimize the basis set on-the-fly and employing ring polymer sampling trajectories to capture tunnelling dynamics. Work has been published in international journals (*The Journal of Chemical Theory and Computation*) and presented at national conferences, winning awards such as the 2016 RSC Coulson Prize.

Durham University, Durham, United Kingdom
MChem (Integrated Master's with Hons) in Chemistry, 2:1 *2009–2013*
Masters thesis: *Electron affinities and overlap dispersion in density functional theory.*
Supervised by Prof. David Tozer. Investigated links between spurious overlap dispersion and trends in electron affinities and ionization potentials within density functional theory.

Publications

- Cavity-Modified Fermi's Golden Rule Rate Constants from Cavity-Free Inputs, M.A.C. Saller, Y. Lai and E. Geva, *J. Phys. Chem. C*, **127** 3154-3164 (2023)
- Quasiclassical approaches to the generalized quantum master equation, G. Amati, M.A.C. Saller, A. Kelly and J.O. Richardson, *J. Chem. Phys.*, **23**, 234103 (2022)
- An Accurate Linearized Semiclassical Approach for Calculating Cavity-Modified Charge Transfer Rate Constants, M.A.C. Saller, Y. Lai and E. Geva, *J. Chem. Phys. Lett.*, **13**, 2330–2337 (2022)
- Benchmarking Quasiclassical Mapping Hamiltonian Methods for Simulating Cavity-Modified Molecular Dynamics, M.A.C. Saller, A. Kelly and E. Geva, *J. Chem. Phys. Lett.*, **12**, 3163-3170 (2021)
- Benchmarking Quasiclassical Mapping Hamiltonian Methods for Simulating Electronically Nonadiabatic Molecular Dynamics, X. Gao, M.A.C. Saller, Y. Liu, A. Kelly, J.O. Richardson and E. Geva, *J. Chem. Theo. Comput.*, **16**, 2883-2895 (2020)
- Path-integral approaches to nonadiabatic dynamics, Book Chapter in *Quantum Chemistry and Excited States: Methods and Applications*, M.A.C. Saller, J.E. Runeson and J.O. Richardson, Wiley, 629–653 (2020)
- Emerging opportunities and future directions: general discussion, *Faraday Discuss.*, **221**, 564–581 (2019)
- Quantum coherence in complex environments: general discussion, *Faraday Discuss.*, **221**, 168-201 (2019)
- Improved population operators for multi-state nonadiabatic dynamics with the mixed quantum-classical mapping approach, M.A.C. Saller, A. Kelly and J.O. Richardson, *Faraday Discuss.*, **221**, 150–167 (2019)
- On the identity of the identity operator in nonadiabatic linearized semiclassical dynamics, M.A.C. Saller, A. Kelly and J.O. Richardson, *J. Chem. Phys.*, **150**, 071101 (2019)
- Quantum Dynamics with Short-Time Trajectories and Minimal Adaptive Basis Sets, M.A.C. Saller and S. Habershon, *J. Chem. Theo. Comput.*, **13**, 3085–3096 (2017)
- Basis Set Generation for Quantum Dynamics Simulations Using Simple Trajectory-Based Methods, M.A.C. Saller and S. Habershon, *J. Chem. Theo. Comput.*, **11**, 8–16 (2015)

Teaching and Service

- **Lecture Courses**, *University of Michigan*
  Teaching undergraduate lecture courses, CHEM 262 - Mathematical Methods for Physical Scientists and CHEM 461 - Physical Chemistry I (Quantum Mechanics), on a substitute basis.
- **Mathematica Workshops**, *ETH Zurich*
  Developing and teaching an introductory undergraduate workshop for the Mathematica software and Wolfram language. Focus on numerical and analytical approaches to scientific problems.
- **Programming Skills for Chemists**, *ETH Zurich*
  Introduction to programming in C/C++, compilation and working in Linux. Focus on establishing programming as a tool first year students can use to solve problems over the course of their degree.
- **Physical Chemistry Tutorials**, *ETH Zurich*
  Leading problem classes with small groups of undergraduate students. Working through topics covered in lectures, contextualizing and deepening understanding. Providing support solving typical exam problems.
- **Masters Research Projects** *University of Warwick*
  Coordinating and supervising 6-month undergraduate research projects. Introduction to programming, working in high-performance computing environments and scientific writing (LaTeX).
- **Computational Chemistry Laboratory Projects**, *University of Warwick*
  Supervising and developing undergraduate computer laboratory projects. Crash course in Linux and terminal environments. Introduction to computational chemistry software culminating in a research project.
- **Spectroscopy in Schools**, *University of Warwick/Royal Society of Chemistry*
  Providing high school students with hands-on experience using portable, research-grade spectroscopy equipment. Providing advice on higher education, particularly in STEM fields.

Awards and Grants

- **ETH Postdoctoral Fellowship 2018–2020** Competitive 24-month postdoctoral fellowship at ETH Zurich.
- **Warwick University Award for Teaching Excellence 2017** Postgraduate teaching commendation.
- **2016 Coulson Prize** Best graduate talk at the RSC Theoretical Chemistry Group Conference 2016.
- **2016 Contributed Talk Prize** RSC Spectroscopy and Dynamics Group Meeting 2016.
- **2016 Talk Prize** University of Warwick, Department of Chemistry Postgraduate Symposium 2016.

Conferences

- **52nd Midwest Theoretical Chemistry Conference**
  Ohio State University, Jun 2022. Contributed talk
- **Faraday Discussion: Quantum effects in complex systems**
  University of Warwick, Sep 2019. Presenting invited article and panel member for general discussion.
- **Recent developments in quantum dynamics, an E-CAM state-of-the-art workshop**
  Lyon, June 2019
- **C4 Computational Workshop**
  University of Zurich, June 2019. Invited talk
- **Computational Molecular Science**
  University of Warwick, March 2019
- **CECAM Workshop: Non-adiabatic quantum dynamics: From theory to experiment**
  University of Lausanne, July 2018

Skills

Research

- Very experienced designing and leading research projects involving multiple researchers.
- Very experienced developing and pursuing independent novel research avenues.
- Experienced developing research projects at the undergraduate and postgraduate level.
- Very experienced supervising and overseeing undergraduate and postgraduate research.
- Very experienced preparing research for publication in international academic journals and grant applications.

Teaching

- Very experienced teaching at both the undergraduate and postgraduate level.
- Experienced creating and presenting undergraduate lectures and lecture courses.
- Very experienced creating and administering workshops and tutorials to undergraduate students.

Computational and Technical

- Ten years experience developing scientific software in Python, Fortran and C/C++.
- Very experienced with parallelisation and optimization for HPC environments.
- Experience assembling and maintaining workstation and server-grade HPC hardware.

Communication and Languages

- Very experienced presenting complicated scientific concepts to both specialist and general audiences.
- Native speaker of English and German. Basic to conversational skills in Japanese.

References

Prof. Eitan Geva	University of Michigan, USA	eitan@umich.edu
Prof. Barry Dunietz	Kent State University, USA	bdunietz@kent.edu
Prof. Aaron Kelly	Dalhousie University, Canada	aaron.kelly@dal.ca
Prof. Jeremy Richardson	ETH Zurich, Switzerland	rjeremy@ethz.ch
Prof. Scott Habershon	University of Warwick, United Kingdom	s.habershon@warwick.ac.uk