David M. G. Williams

Curriculum Vitae

Personal Information

Full Name David Mounir Günter Williams

Date of Birth 04/26/1992

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Research Positions

Jan. 2022 – Present

Stanford University

Postdoctoral researcher in the group of Prof. Todd Martínez

Jan. 2021 – Dec. 2021

Bielefeld University

Postdoctoral researcher in the group of Prof. Dr. Wolfgang Eisfeld

Education

2016 – Jan. 2021 **Doctor rerum naturalium, PhD**
Theoretical Chemistry, Bielefeld University, Germany
Thesis: "Conquering coupled diabatic potential energy surfaces with artificial neural networks for nonadiabatic dynamics"

2014 – 2016 **Master of Science**
Theoretical Chemistry, Bielefeld University, Germany
Thesis: "Neural Network Based Methods for the Representation of Diabatic Potential Energy Surfaces"

2011 – 2014 **Bachelor of Science**
Chemistry, Bielefeld University, Germany
Thesis: "Das Konzept der Hybrid-Diabatisierung am Beispiel von Ozon"

2011 **Graduation**
Abitur (upper secondary education), Gymnasium Leopoldinum, Detmold

Research Interests

- Molecular quantum dynamics of excited states
- Numerical method development based on artificial neural networks
- Efficient, modularized models of complex systems
- Data-driven analysis and method development

Technical Skills

Programming languages	Proficient in Fortran, working experience with Python, Bash, and various Lisp dialects
2016 – 2021	Assistant System Administrator – Responsible for queueing system, software deployment, and account management for the Theoretical Chemistry Department, Bielefeld University
2019 – Present	Contributor to and maintainer of various free software projects

Peer-Reviewed Publications

1. A. Viel, **D. M. G. Williams**, and W. Eisfeld,
   Accurate quantum dynamics simulation of the photodetachment spectrum of the nitrate anion (NO_3^-) based on an artificial neural network diabatic potential model,
   J. Chem. Phys. **154**, 084302 (2021).

2. **D. M. G. Williams** and W. Eisfeld,
   Complete nuclear permutation inversion invariant artificial neural network (CNPI$\bar{I}$ANN) diabatization for the accurate treatment of vibronic coupling problems,
   J. Phys. Chem. A, **124**, 7608-7621 (2020)

3. **D. M. G. Williams**, A. Viel, and W. Eisfeld,
   Diabatic neural network potentials for accurate vibronic quantum dynamics– The test case of planar NO_3, J. Chem. Phys. **151**, 164118 (2019)

4. T. Weike, **D. M. G. Williams**, A. Viel, and W. Eisfeld,
   Quantum dynamics and geometric phase in $E \otimes e$ Jahn-Teller systems with general C_{nv} symmetry, J. Chem. Phys. **151**, 074302 (2019)

5. **D. M. G. Williams** and W. Eisfeld,
   Neural network diabatization: A new ansatz for accurate high-dimensional coupled potential energy surfaces, J. Chem. Phys. **149**, 204106 (2018)

6. N. Wittenbrink, F. Venghaus, **D. M. G. Williams** and W. Eisfeld,
   A new approach for the development of diabatic potential energy surfaces: Hybrid block-diagonalization and diabatization by ansatz., J. Chem. Phys. **145**, 184108 (2016)

Conference Contributions and Meetings

Aug. 2017	**Symposium on Theoretical Chemistry** Poster, "Neural Network Diabatization: A new ansatz for high-dimensional coupled potential energy surfaces" *Basel, Switzerland*
Aug. 2018	**22nd European Conference on the Dynamics of Molecular Systems** Poster, "Accurate vibronic quantum dynamics of NO_3 using a diabatic neural network potential" *Dinard, France*
Apr. 2021	**Online Seminar at the IPR (Institute of Physics Rennes)** "Conquering coupled diabatic potential energy surfaces with artificial neural networks for nonadiabatic dynamics" *Rennes, France*

Teaching Experience

Teaching Assistant	Advanced Theoretical Chemistry II	(M.Sc. Chem. tutorial)
	Computational Chemistry I	(M.Sc. Chem. lab)
	Computational Chemistry II	(M.Sc. Chem. lab)
	Theoretical Chemistry I	(B.Sc. Chem. tutorial)
	Mathematics for Chemists I	(B.Sc. Chem. tutorial)
	Mathematics for Chemists II	(B.Sc. Chem. tutorial)
Co-Supervisor	Bachelor thesis	
	Programming – Molecular Structure	(M.Sc. Chem. lab)