

Dr. Christoph Schran

Professional Experience

Since 10/2020	PostDoc @ Yusuf Hamied Department of Chemistry, University of Cambridge, UK & Department of Physics and Astronomy, UCL, UK
09/2020–01/2020	PostDoc @ Department of Physics and Astronomy, UCL, UK “Machine Learning Potentials for Complex Aqueous Systems” with Prof. A. Michaelides Feodor Lynen fellow of the Alexander von Humboldt Foundation (2020-2022) Walter Benjamin fellow of the German Research Foundation (since 10/2022)
12/2019 – 10/2019	PostDoc @ Faculty of Mathematics and Physics, Charles University, Czech Republic “Committee Neural Network Potentials” with Dr. O. Marsalek
09/2019 – 01/2016	PhD student @ Center for Theoretical Chemistry, Ruhr-Universität Bochum, Germany PhD thesis on “Properties of Hydrogen Bonding at Ultra-Low Temperatures in Superfluid Quantum Solvents”, Supervisor: Prof. D. Marx, Graduation with distinction Member of the Graduate School <i>Solvation Science</i> of the Cluster of Excellence <i>RESOLV</i> Fellow of the “Studienstiftung des Deutschen Volkes” & “Verband der Chemischen Industrie”
08/2017 – 05/2017	Visiting graduate student @ École Normale Supérieure, Paris, France “Quantum Dynamics via the Phase Integration Method” with Prof. R. Vuilleumier Supported by a travel grant of the German Research Foundation
08/2015 – 01/2015	Visiting graduate student @ Stanford University, Palo Alto, USA Master thesis on “Nuclear Quantum Effects on the Electronic Properties of the Hydrogen Bond” with Prof. T. Markland in cooperation with Prof. D. Marx, Grade: 1.0* Supported by a travel grant of the “Studienstiftung des Deutschen Volkes”

Education

09/2015 – 10/2013	Master of Science in Chemistry @ Ruhr-Universität Bochum, Germany GPA: 1.0*, best graduate of the year (ranking: 1/38) Prize of the Ruhr-Universität for best graduate of the Faculty of Chemistry and Biochemistry Fellow of the “Studienstiftung des Deutschen Volkes” & “Bildungsfond der Ruhr-Universität”
09/2013 – 10/2010	Bachelor of Science in Chemistry @ Ruhr-Universität Bochum, Germany GPA: 1.0*, best graduate of the year (ranking: 1/55) August-Wilhelm-von-Hofmann fellow of the German Chemical Society
12/2012 – 09/2012	Exchange Semester @ University of Glasgow, Scotland Supported by a travel grant of the Erasmus programme

Teaching and Supervision

Since 10/2022	Lecture course (12 lectures) on <i>Frontiers of Atomistic Simulation Techniques</i> in the Natural Sciences Tripos Part III Chemistry, University of Cambridge, UK
Since 10/2020	Senior demonstrator & supervisions for Clare College in the Natural Sciences Tripos Part IB Chemistry A, University of Cambridge, UK
Since 01/2020	Supervision of PhD students (Patrick Rowe, Fabian L. Thiemann, Niamh O’Neill) in the group of Prof. A. Michaelides, University of Cambridge & University College London, UK
09/2019 – 10/2011	Teaching assistant @ Center for Theoretical Chemistry, Ruhr-Universität Bochum, Germany Supervision of Bachelor and Master student projects and weekly tutorials

*) Academic grading in Germany: excellent (1.0) - insufficient (5.0)

Volunteering Work

Since 08/2021	Co-organizer of the Lennard-Jones Centre Discussion Group, University of Cambridge Organization of weekly seminars with focus on molecular simulations
Since 06/2021	Member of the management board of the Lennard-Jones Centre, University of Cambridge Connecting researchers within Cambridge with interest in materials modelling
09/2019 – 01/2014	Member and Vice-Speaker (2018–2016) of the “Young Chemist Association” Bochum Organisation of lectures, workshops, and events for students and the general public on topics such as the “disposal of chemical weapons in Syria”, or “sustainability in science”

5 Key Publications (out of 21)

- [1] *The first-principles phase diagram of monolayer nanoconfined water*
V. Kapil, **C. Schran**, A. Zen, J. Chen, C. J. Pickard, A. Michaelides
Nature, **2022**, 609, 512-516
- [2] *Water Flow in Single-Wall Nanotubes: Oxygen Makes It Slip, Hydrogen Makes It Stick*
F. L. Thiemann, **C. Schran**, P. Rowe, E. A. Müller, A. Michaelides
ACS Nano, **2022**, 16 (7), 10775-10782
- [3] *Machine learning potentials for complex aqueous systems made simple*
C. Schran, F. L. Thiemann*, P. Rowe*, E. A. Müller, O. Marsalek, A. Michaelides
Proc. Nat. Acad. Sci., **2021**, 118 (38), e2110077118
- [4] *Committee neural network potentials control generalization errors and enable active learning*
C. Schran, K. Brezina, O. Marsalek, *J. Chem. Phys.*, **2020**, 153 (10), 104105
- [5] *Automated Fitting of Neural Network Potentials at Coupled Cluster Accuracy: Protonated Water Clusters as Testing Ground*
C. Schran, J. Behler, D. Marx, *J. Chem. Theory Comput.*, **2020**, 16 (1), 88-99

(* = equal contribution, ____: corresponding author)

Additional Qualifications

Funding	Post-Graduate
Since 10/2020	Walter Benjamin fellowship of the German Research Foundation (~84,000€)
01/2020–03/2022	Feodor Lynen fellowship of the Alexander-von-Humboldt Foundation (~91,000€)
	Graduate
11/2016–10/2018	Studienstiftung des Deutschen Volkes (~52,000€)
11/2016–07/2018	Verband der Chemischen Industrie (~45,000€)
	Undergraduate
10/2014–09/2015	Studienstiftung des Deutschen Volkes (~3,600€) including travel grant (~9,000€)
10/2013–09/2014	Bildungsfond of the Ruhr-Universität Bochum (~3,600€)
04/2012–09/2013	August-Wilhelm-von-Hofmann scholarship of the German Chemical Society (~5,400€)

Prizes and Awards

10/2022	Short-listed for TYC Early Career Award
Since 10/2021	College Research Associate at Clare College, University of Cambridge
12/2016	Prize of the Ruhr-Universität for “best graduate of the Faculty of Chemistry and Biochemistry”

Languages	Programming and HPC	Interests
German (native)	Fortran, python, bash, MPI/OpenMP	Handball
English (fluent)	CP2K developer	Beer brewing

I have arranged for the following three referees to be contacted during the course of the application process:

- **Prof Angelos Michaelides**, Yusuf Hamied Department of Chemistry, University of Cambridge, Lensfield Rd, Cambridge CB2 1EW, UK, E-mail: am452@cam.ac.uk
- **Prof Dominik Marx**, Center for Theoretical Chemistry, Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum, Germany, E-mail: dominik.marx@rub.de
- **Prof Thomas E. Markland**, Department of Chemistry, Stanford University, 364 Lomita Drive Stanford, CA 94305, USA, Email: tmarkland@stanford.edu.