

## Roman Ellerbrock



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**Date of Birth** 5/27/1990

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## Research Positions

**2019 – present** **Postdoctoral researcher** in the group of Prof. Todd Martinez

**2018 – 2019** **Postdoctoral scholar** in the group of Prof. Dr. Uwe Manthe

## Education

**2014 – 2018** **Doctor rerum naturalium**, chemistry  
Doctoral study in the group of Prof. Dr. Uwe Manthe  
Bielefeld University  
Title of thesis: “State-resolved reactivity of methane and its isotopic analogues”  
Grade: *summa cum laude*

**2012 – 2014** **Master of Science**, theoretical chemistry  
Study of chemistry in Bielefeld, Germany  
Thesis: “Quantum State-resolved reactivity in the  $\text{H}+\text{CHD}_3 \rightarrow \text{H}_2+\text{CD}_3$  reaction”  
In the group of Prof. Dr. Uwe Manthe  
Grade of thesis: **1.0 (best possible)** final grade: **1.0 (best possible)**

**2009 – 2012** **Bachelor of Science**, chemistry  
Study of chemistry in Bielefeld University, Germany  
Thesis: “ $\text{SF}_6$ : A 15-dimensional potential energy surface based on modified Shepard Interpolation” in the group of Prof. Dr. Wolfgang Eisfeld  
Grade of thesis: **1.0 (best possible)** final grade: **1.3** (on a scale of 1.0 (best) to 5.0)

## Awards

### Price of the Friedrich-Wilhelm Helweg Foundation

Award for outstanding master’s degree 2014 | Given to one chemistry student at Bielefeld University per year  
Awarded with 2000 Euro

## Talks on Conferences and Meetings

**2019 (expected)** **Invited talk** on the **Quantum Reactive Scattering (QRS2019)** conference,  
Saitama University, Japan

**Sep. 2018** **Invited talk** on the **High-Dimensional Quantum Dynamics (HDQD2018)** conference,  
Lille, France

**Nov. 2017** “Initial State-Selected Reaction Probabilities for the  $\text{H}+\text{CHD}_3 \rightarrow \text{H}_2+\text{CD}_3$  Reaction”,  
Talk in the group of Profs. Todd Martinez  
Stanford University, Stanford, USA

## Research visits

**April – June 2016** **University of Quilmes**, Buenos Aires, Argentina  
Research visit in the group of Prof. Juliana Palma

## Peer-Reviewed Publications

1. **Roman Ellerbrock** and Uwe Manthe  
“Natural Reaction Channels in  $H+CHD_3 \rightarrow H_2+CD_3$ ”, Faraday Discuss. 212, 217-235 (2018)
2. **Roman Ellerbrock** and Uwe Manthe  
“Full-dimensional quantum dynamics calculations for the  $H+CHD_3 \rightarrow H_2+CD_3$  reaction: The effect of multiple vibrational excitation”, J. Chem. Phys, 148 (22), 224303 (2018)
3. **Roman Ellerbrock** and Uwe Manthe  
“Communication: Reactivity borrowing in the mode selective chemistry of  $H+CHD_3 \rightarrow H_2+CD_3$ ”, J. Chem. Phys., 147 (24), 241104 (2017)
4. **Roman Ellerbrock** and Uwe Manthe  
“ $H+CH_4 \rightarrow H_2+CH_3$ : Initial State-Selected Reaction Probabilities on Different Potential Energy Surfaces”, Chemical Physics 482, 106-112 (2017)
5. Uwe Manthe and **Roman Ellerbrock**  
“S-matrix decomposition, natural reaction channels and the quantum transition state approach to reactive scattering”, J. Chem. Phys, 144 (20), 204119 (2016)

## Software Development & Programming Skills

2017 – present **Main developer of mctdh++:**

A modern C++ implementation of the **multilayer multi-configurational time-dependent Hartree (MCTDH)** approach including:

- the multilayer correlation discrete variable representation (**CDVR**)
- the constant mean-field (**CMF**) approach
- time-dependent discrete variable representation (**TDDVR**)
- weighted simultaneous diagonalization (**WSD**)
- Iterative eigenstate calculation via **Lanczos** approach & via **Block relaxation**
- an efficient library for Tensor operations in density-based approaches (**QDlib**)

2014 – 2018 **Assistant System Administrator**

Responsible for file servers, Computation Cluster & Queueing system of the Chemistry department, Bielefeld University

2016 **NVIDIA CUDA** programming course for scientific computing on GPUs

CUDA Projects: Implementing highly optimized linear algebra functions, Ising Models and modular feed-forward neural networks on GPUs

**Programming** Proficient in modern C++, C, CUDA and Fortran

## Teaching Experience

<b>Teaching Assistant</b>	Advanced Theoretical Chemistry II	(MSc. Chem. lecture)
	Advanced Theoretical Chemistry I	(MSc. Chem. lecture)
	Programming – Standard Wave Packet Dynamics	(MSc. Chem. course)
	Theoretical Chemistry II	(MSc. Chem. lecture)
	Theoretical Chemistry I	(MSc. Chem. lecture)
	Computational Chemistry II	(MSc. Chem. lecture)
	Computational Chemistry I	(MSc. Chem. lecture)
	Mathematics for Chemists II	(MSc. Chem. lecture)
	Mathematics for Chemists I	(MSc. Chem. lecture)
	Co-Supervision of a master’s thesis	