

# JESSICA DE RUITER

MSc Chemistry, PGCertSci Physics

SCIENCE • COMMUNICATION • SUSTAINABILITY • DIVERSITY

## Objective

I am looking for a team in which I can facilitate cross-disciplinary communication and problem solving, in a company that prioritises sustainability.

## Profile

The driving force behind my computational chemistry PhD is my desire to contribute to a sustainable future. I am interested in how science may be communicated within the business sector, as well as using scientific thought processes to engage and perform more effectively. Throughout my experiences I have concluded that one of the keys to a team's sustainability is its diversity, and as such am a strong advocate for diversity within the workplace.

## Skills

Quick to learn new computational tools

Logical and structured thinker

⇒ Short project start-up time

Able to explain complex concepts in simple language

Can adapt easily to a specific audience

Invested in two-way communication

⇒ Business – client communication

Clear and concise writing style

Successful in collecting and distilling information

⇒ Written summaries, publishable content

Reliable and committed

Highly motivated to reach key objectives

⇒ Solutions

Can cooperate in groups both as a leader and contributing follower

⇒ Adaptable and mobile employee

## Experience

2013 - present

Universiteit Leiden

Leiden, NL

### PhD Researcher

Research using a number of different computational chemistry techniques in order to better understand water oxidation catalysts. These catalysts are a step towards sustainable fuels.

See also Scientific Appendix

Feb – Aug 2012

Philips Research

Eindhoven, NL

### Research Intern

Responsible for DDFT based modelling of the self-assembly of block copolymers in templates of different size. Part of a multidisciplinary team focussed on developing solutions for a client, to whom results had to be communicated in a clear and succinct way.

Nov 2010 – Feb 2011

Industrial Research Ltd

Lower Hutt, NZ

### Summer Intern

Computational solid state chemistry research project examining the size-dependent transition of nanoparticles from having molecular properties to metallic properties.

2003 – 2013

Various part time jobs including music school evening concierge (2 years), university homework marker, house keeper, Subway employee (5 years).

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## Education

2011 – 2013

Universiteit Leiden

Leiden, NL

### Master of Science in Chemistry, *cum laude*

Research specialisation focussing on Theoretical Chemistry, with a research component GPA 9.

2011

Victoria University of Wellington

Wellington, NZ

### Postgraduate Certificate of Science in Physics

Including 5 month palaeomagnetism research project “Characterising carriers of magnetic remanence in New Zealand sands”. GPA 7.8.

2008, 2010

Victoria University of Wellington

Wellington, NZ

### Bachelor of Science in Physics and Chemistry

Courses completed in physics, math, chemistry and statistics. GPA 7.8.

2009

Rijksuniversiteit Groningen

Groningen, NL

### University Exchange

Courses completed in physics, math and chemistry, taking 125% of the nominal course load.

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## Volunteer Experience & Leadership

- TopFem Advisory Board, TopFem Webmaster, TopFem Board
- Kiwi Ranch Curious Cove Holiday Camp Children’s Camp Leader
- TopFem Talent Programme
- Victoria International Leadership Programme

See also Volunteer and Leadership Appendix

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### Software

Linux, BASH, Fortran  
CPMD, ADF, CP2K  
Gaussian, Culgi, CRYSTAL  
MS Office, Origin, VMD

### Languages

English, Dutch  
Rudimentary French

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### Courses & Training

2011 – present  
Emergency Response officer

2014  
Communication in Science  
(2 ECTS Leiden University)

2015  
Introduction to teaching for PhD  
Students  
(1 ECTS ICLON, Leiden University)

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### Extracurricular

2014 - present  
ISN Leiden Theatre Group

2013 – present  
TopFem Network

2013 – 2014  
Leiden Debating Union

2009  
T.F.V. ‘Professor Francken’

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### Appendices to this CV

Scientific  
Volunteering and Leadership

# SCIENTIFIC APPENDIX

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## Current Research

In the search for sustainable energy solutions, the idea of artificial photosynthesis has been proposed as a sustainable means of using water and sunlight to produce fuels (for example hydrogen). Key in the development of such technologies is the splitting of water using a water oxidation catalyst.

In my research I investigate the water splitting catalytic process using a number of different computational techniques. I use DFT to calculate spectroscopic and electrochemical properties which can then be compared to experimental observables. Because these catalytic processes are dynamic, I also investigate catalysts in a fully solvated system with CPMD. Combining these techniques gives us a better idea of the things needed in the optimisation of water oxidation catalysts.

Most recently I have been devising a novel approach with which one can examine the dynamic transition from one catalytic intermediate to another. Traditionally these transitions have been considered statically, with approaches that often include a number of correction factors. In the new approach all the charge carriers (which are usually corrected for) are included in a dynamic simulation.

## Publications

J. M. de Ruiter, R. L. Purchase, A. Monti, C. J. M. van der Ham, M. P. Gullo, K. S. Joya, M. D'Angelantonio, et al. "Electrochemical and Spectroscopic Study of Mononuclear Ruthenium Water Oxidation Catalysts: A Combined Experimental and Theoretical Investigation." *ACS Catalysis*, **2016**, doi: 10.1021/acscatal.6b02345

J. M. de Ruiter, and F. Buda "Introducing a Closed System Approach for the Investigation of Chemical Steps Involving Proton and Electron Transfer; as Illustrated by a Copper-Based Water Oxidation Catalyst." *Physical Chemistry Chemical Physics*, **2016**, doi: 10.1039/C6CP07454E

A. Monti, J. M. de Ruiter, H. J. M. de Groot, and F. Buda. "A Dynamic View of Proton-Coupled Electron Transfer in Photocatalytic Water Splitting." *The Journal of Physical Chemistry C*, **2016**, doi:10.1021/acs.jpcc.6b08244.

H. Boots, J. M. de Ruiter, T. T. Nguyen, A. Brizard, E. Peeters, S. F. Wuister, T.S. Druzhinina, J. K. Wolterink, J. G. E. M. (Hans) Fraaije. "Pitch Variations of Self-Assembled Cylindrical Block Copolymers in Lithographically Defined Trenches." *J. Micro/Nanolith. MEMS MOEMS* **2014**, doi:10.1117/1.JMM.13.3.033015.

T. T. Nguyen, J. M. Finders, W. S. M. M. Ketelaars, S. F. Wuister, E. C. A. van der Heijden, H. J. C. Meessen, R. Koole, E. Peeters, C. M. van Heesch, A. Brizard, H. Boots, T. S. Druzhinina, J. M. de Ruiter, "Method to provide a patterned orientation template for a self-assemblable polymer." ASML Netherlands B.V, *US Patent App. 20140245948*, filed 2 Oct 2014, and published 4 Sep 2014.

## Conferences

Dec 2016	CHAINS	Veldhoven
	Presentation “A closed system approach to investigate the catalytic cycle of a copper water oxidation catalyst.”	
Nov 2016	Annual HRSMC Symposium	Leiden
	Poster “A Combined Theoretical And Experimental Investigation Of Mononuclear Ruthenium Water Oxidation Catalysts.”	
Aug 2016	The 17 <sup>th</sup> International Congress on Photosynthesis Research	Maastricht
	Presentation and poster “A closed system approach for the in-depth investigation of catalytic steps, as illustrated by a copper based water oxidation catalyst.”	
Dec 2015	CHAINS	Veldhoven
	Poster “A closed system investigation of the oxygen - oxygen bond formation for a copper-based water oxidation catalyst.”	
Nov 2015	Annual HRSMC Symposium	Amsterdam
	Poster as above	
June 2015	BioSolar Cells Annual Meeting	Wageningen
	Poster “The active species in water splitting: Monomers vs. dimers and the interpretive role of computational chemistry.”	
Nov 2014	CHAINS	Veldhoven
	Poster “Closing The Box: A Closed System Approach To The Theoretical Examination Of A Catalytic Step.”	
Nov 2014	Annual HRSMC Symposium	Amsterdam
	Poster as above	
June 2014	BioSolar Cells Annual Meeting	Wageningen
	Poster and poster flash presentation “Electrochemical and Optical Study of Mononuclear Ruthenium Water Oxidation Catalysts: A Combined Experimental and Theoretical Investigation.”	
Nov 2013	Annual HRSMC Symposium	Leiden
Nov 2013	Lorentz Workshop ‘Responsive Matrices for Solar Fuels’	Leiden

## Teaching

2015, 2016	Lab Assistant Chemistry Apparatus Room for First Year Students
2015	Supervisor Chemistry Internship First Year Student

## Awards

2016	Poster prize winner Theme 1, Annual HRSMC Symposium
2016	Poster prize finalist, HRSMC Photochemistry School



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## Schools

Aug 2016	HRSMC Photochemistry School 2 ECTS	Maastricht
Jan 2015	CECAM Understanding Molecular Simulation School 3 ECTS	Amsterdam
April 2014	HRSMC Photophysics, Photochemistry & Photobiology school 3 ECTS	Amsterdam
Dec 2013	UvA Winter School for Theoretical Chemistry and Spectroscopy 2 ECTS	Han-sur-Lesse

# VOLUNTEERING & LEADERSHIP APPENDIX

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## Volunteering & Leadership

- 2016 – present      TopFem      Amsterdam, NL  
**Advisory Board**  
Involved in cementing current vision for the network, advising current board.
- 2015 – present      TopFem      Amsterdam, NL  
**Webmaster**  
Internationalised and redesigned the TopFem website, responsible for network-wide profile and e-mail account management as well as website upkeep and expansion.
- 2015 – 2016      TopFem      Amsterdam, NL  
**Board Member in Charge of Marketing**  
Developed and structured the online presence of the TopFem network, including development of style guidelines and publication protocols. Chair of the TopFem Marketing Committee.
- 2006 – 2011      Kiwi Ranch Curious Cove Holiday Camp      Picton, NZ  
**Children's Camp Leader**  
Providing primary care for a group of ten 11 to 14 year olds at a boat-access only, week long children's camp. Often assigned 'problem' children or co-leaders.
- 2009      T.F.V. 'Professor Francken'      Groningen, NL  
**Secretary Annual Symposium Committee**  
Responsible for communicating with external parties, inviting speakers and taking minutes. Having never been taught how to write Dutch, this greatly improved my written Dutch. At my suggestion the scope of the speakers invited was broadened. This symposium was the 2<sup>nd</sup> most successful of the decade.
- 2007      Marlborough Girls' College      Blenheim, NZ  
**Academic Prefect**  
Initiated and set-up a number of academic activities, liaising with the two Marlborough Boys' College Academic Prefects. Coordinated a school-wide (1000 girls) voluntary tutoring system. Chair of the Academic Committee.



## Leadership Programmes

2013 – 2014

TopFem

Amsterdam, NL

### **TopFem Talent Programme**

*Talent of the Year 2014*

A programme comprised of three main pillars: participation in the networking aspect of TopFem, self-development, and an internship at a company or ministry.

Research performed via interviews with various employees at AkzoNobel, culminating in “*A girl’s guide to AkzoNobel: A commentary on being a female science graduate at AkzoNobel.*”

2008, 2010

Victoria University of Wellington

Wellington, NZ

### **Victoria International Leadership Programme**

An academically-oriented extra-curricular programme of seminars, speaker events and experiential activities relevant to the themes of international leadership, cross-cultural communication, global connectedness and sustainability.