



Universiteit
Leiden
The Netherlands

Observing what cannot be observed: computational electrochemistry from carbon to hydrogen

Hanselman, S.R.

Citation

Hanselman, S. R. (2022, December 20). *Observing what cannot be observed: computational electrochemistry from carbon to hydrogen*. Retrieved from <https://hdl.handle.net/1887/3503522>

Version: Publisher's Version

License: [Licence agreement concerning inclusion of doctoral thesis in the Institutional Repository of the University of Leiden](#)

Downloaded from: <https://hdl.handle.net/1887/3503522>

Note: To cite this publication please use the final published version (if applicable).

List of publications

Publications listed in thesis

Chapter 2

Hanselman, S.; Koper, M. T. M.; Calle-Vallejo, F. Computational Comparison of Late Transition Metal (100) Surfaces for the Electrocatalytic Reduction of CO to C₂ Species. *ACS Energy Letters* **2018**, 3(5):1062–1067.

Chapter 4

Hanselman, S.; Koper, M. T. M.; Calle-Vallejo, F. Trends in adsorbed hydroxyl – water interactions on late transition metal nanoparticles. *Physical Chemistry Chemical Physics* (in revision).

Chapter 5

Arulmozhi, N.; Hanselman, S.; Viorica, T.; Chen, X.; van Velden, D.; Schneider, G.; Calle-Vallejo, F.; Koper, M. Energetics and kinetics of hydrogen electrosorption on a graphene-covered Pt(111) electrode. *JACS Au* (in revision).

Chapter 6

Hanselman, S.; Calle-Vallejo, F.; Koper, M. T. M. Computational description of surface hydride phases on Pt(111) electrodes. *Journal of Chemical Physics* (in revision).

Chapter 7

Hanselman, S.; McCrum, I. T.; Rost, M. J.; Koper, M. T. M. Thermodynamics of the formation of surface PtO₂ stripes on Pt(111) in the absence of subsurface oxygen. *Physical Chemistry Chemical Physics* **2020**, 22:10634–10640.

Other publications

He, Z. D.; Hanselman, S.; Chen, Y. X.; Koper, M. T. M.; Calle-Vallejo, F. Importance of Solvation for the Accurate Prediction of Oxygen Reduction Activities of Pt-Based Electrocatalysts. *Journal of Physical Chemistry Letters* **2017**, 18(8,10):2243–2246.

Acknowledgements

During my time as an MSc student and PhD candidate at our CASC group, I have met many fantastic fellow scientists and dear colleagues – unfortunately, too many to be listed within any reasonable number of pages. I will hereby mention some people who were directly involved in my research and scientific work, but also in my non-academic life.

Firstly, I wish to thank Marc Koper for his support before and during my PhD time at CASC. Long before I would become part of the PhD community at Leiden University, you helped spark my interest in physical chemistry, and supported my efforts to broaden my scientific horizon during my MSc years – whether it concerned solar fuels, applied physics, or computational chemistry. Your support during my MSc internship convinced me to join the wonderful world of academia on your behest, which I still do not regret. Federico Calle-Vallejo, you contributed just as greatly to my decision to board the PhD boat onto the seas of science. Your support during my MSc internship taught me what I need to know about academia, and the philosophy of science and popular culture if we felt like discussing it. Fortunately, we would meet again at the Universitat de Barcelona for my HPC-Europa3 project! Living on my own for the first time, far from home, in a world overwhelmed by unprecedented conditions (which would eventually cut short my stay), you provided the support I needed to thrive scientifically. Good luck in San Sebastián! José, you were really helpful during my stay at CASC, and we had great conversations, ranging from life at university through sports to classical music. I hope you enjoy your life after employment! Katharina, as fellow computational chemists with a background in physics we could always have good discussions about work, but we also shared another passion: string instruments! Our violin-viola duets were great fun to play, and were hopefully enjoyable to those in the office after 5 pm too. Thom, you were there since my BSc and always were there for a chat – first at the student association, and later at the lunch table at CASC. We had some great stuff done together, even if you had to get out of bed early in California... Nakkiran, thanks for the collaboration on graphene-covered Pt(111); it was a blast. Ian, Laura, Tim, thanks for all the conversations about – and collaborations on – computational chemistry, and being great colleagues. I would also like to thank all my BSc students for their curiosity, hard work, and that I could introduce them into my less immediately obvious subfield of chemistry. A special mention goes to Lucas, whom I supervised for several months in 2021 – video calls are not entirely conducive towards advanced learning, but you nonetheless managed to find many interesting results and write a nice thesis; hope you enjoy your time in Utrecht! Also special thanks to my former CASC roommate Christoph and Akansha, and of course everyone else in the CASC group. Your presence made being a PhD candidate so much more fun.

Caroline, we have known each other pretty much our entire lives, and thanks for being there for me all those years! Sander, since we met during our BSc years, we had the most interesting conversations (and cycling trips), and eventually came to share the PhD experience. I'm really glad you both are in my life.

Above all, I would like to thank Dennis and my parents. Dennis, you have been there for me since before I started at CASC, and helped me stay happy even during the toughest times. Although we are different in terms of academic fields – tax law isn’t quite computational chemistry – we share so much otherwise. I was truly blessed with you having lived in Zoetermeer for a few months, since that mere coincidence was what brought us together. Mom, dad, you have been there since I was born, and provided me with everything I needed to grow into an independent person, and a research scientist to boot. Speaking about research, good luck Dad with the final phase of your own PhD candidacy at the Faculty of Governance and Global Affairs – maybe we will have two PhDs in our family fairly soon!

Curriculum vitae

Selwyn Ragnar Hanselman was born on 4 January 1994 in Zoetermeer, the Netherlands. After completing bilingual VWO cum laude with IB English A2 at Alfrink College, Zoetermeer, he enrolled in the Molecular Science & Technology BSc programme at Leiden University and Delft University of Technology in 2010, majoring in Chemistry and minoring in Politics: Conflict and Consensus (Leiden University). During this time, he successfully completed the Honours College (Leiden University) programme on Bèta & Life Sciences. He completed his BSc programme with an internship at Inorganic Chemistry (Leiden University), supervised by Sylvestre Bonnet, on red-to-blue upconversion in liposomes.

Following his BSc graduation in 2013, he enrolled in two MSc programmes: Applied Physics at Delft UT, and Chemistry at Leiden University. Within the Applied Physics MSc programme, he specialised in nanotechnology with courses including solid-state physics, quantum mechanics, particle physics, and their applications in nanoscopic devices. He subsequently did a research internship at Biophysical Structural Chemistry (Leiden University) and ImPhys (Delft UT) into the simulation of electron trajectories for scanning electron microscopy (SEM) in the Medipix3 pixel detector using Geant4, supervised by Jan Pieter Abrahams and Harry van der Graaf, on which he graduated in 2016. Within the Chemistry MSc programme, he specialised in physical and theoretical chemistry in the context of the NIOK Solar Fuels Catalysis (SFC) graduate school programme (Leiden University, Twente University, Utrecht University, Eindhoven UT), with courses including photocatalysis, theoretical chemistry, and electrochemistry. He did a research internship at Catalysis and Surface Chemistry (CASC) at Leiden University, supervised by Marc Koper and Federico Calle-Vallejo, on the overpotentials of electrochemical CO reduction to C₂ products on late transition metal (100) surfaces, which he completed in 2017. Following this internship, he completed a literature study on recent developments in density functional theory (DFT), after which he graduated in 2017.

He continued his research in 2017 as a PhD candidate at the Koper group, again using DFT to study electrochemical phenomena. Most of these PhD research projects were supported by NWO in the context of the SFC graduate school. He attended the 2017 Winter school on Theoretical Chemistry and Spectroscopy in Han-sur-Lesse (Belgium), and subsequently attended the 2018 CAMD Summer School on Electronic Structure Theory and Materials Design in Helsingør (Denmark). In 2020, he received an HPC-Europa3 grant to study hydrogen adsorption at graphene-covered Pt(111) surfaces at the IQTC (University of Barcelona), supervised by Federico Calle-Vallejo. Results of these projects, including those published in peer-reviewed journals, are listed in this thesis.