

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

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List of publications

Publications listed in thesis

Chapter 2

<u>Hanselman, S.</u>; 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

<u>Hanselman, S.</u>; 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.; <u>Hanselman, S.</u>; 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

<u>Hanselman, S.</u>; 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

<u>Hanselman, S.</u>; 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.; <u>Hanselman, S.</u>; 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.

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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.