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Getting the electrons right for O₂-on-metal systems

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Lijst van Nederlandstalige afkortingen, acroniemen en symbolen

Lijst van afkortingen, acroniemen en symbolen die in het Nederlands anders zijn dan in het Engels. De andere afkortingen zijn in het Engels en Nederlands hetzelfde. Zie 'List of abbreviations, acronyms, and symbols' voor diezelfde afkortingen.

BOB:	<i>Born-Oppenheimer benadering</i>
BOSO:	<i>Born-Oppenheimer statisch oppervlakte</i>
E_{Lo}:	<i>Ladingsoverdrachtenergie</i>
GGB:	<i>Gegeneraliseerde gradiënt benadering</i>
GRP:	<i>Golvingsreductieprocedure</i>
mGGB:	<i>Meta-GGB</i>
NZCV:	<i>Niet-zelfconsistent-veld</i>
PEO:	<i>Potentieel energie-oppervlak</i>
QKB:	<i>Quasi-klassieke baanberekeningen</i>
UC-DF:	<i>Uitwisseling-en-correlatie dichtheidsfunctionaal</i>
ZCV:	<i>Zelfconsistent-veld</i>

Curriculum vitae

Robert A. B. van Bree is geboren op 25 juni 1997 te Haarlem. Op 11 juni 2015 heeft hij zijn VWO diploma gehaald aan het Rijnlands Lyceum Oegstgeest in Oegstgeest. In datzelfde jaar is hij begonnen aan de Bachelor opleiding Molecular Science and Technology aan zowel de Universiteit Leiden als de TU Delft. In de Bachelor heeft hij zijn BSc. verslag geschreven over onderzoek aan experimentele oppervlaktechemie gedaan bij dr. Ludo B. F. Juurlink en dr. Sabine V. Auras in de groep “Catalysis and Surface Chemistry”, aan de Universiteit Leiden. Op 31 juli 2018 heeft hij deze opleiding *Cum Laude* afgerond en is direct daarna begonnen aan zijn Master opleiding “Chemistry” aan de Universiteit Leiden. Tijdens deze opleiding heeft hij een literatuuronderzoek gedaan betreffende de elektrolyse van zeewater onder begeleiding van prof. dr. Marc T. M. Koper bij “Catalysis and Surface Chemistry”. Zijn MSc. verslag betrof het fitten van een analytisch EAM model voor Cu(111), het onderzoek is gedaan en het verslag geschreven onder begeleiding van dr. Mark F. Somers en dr. Bauke Smits in de Theoretische Chemiegroep aan de Universiteit Leiden. Het MSc. diploma heeft hij op 30 oktober 2020 *Cum Laude* behaald. Per 1 November 2020 is hij begonnen aan zijn promotieonderzoek onder begeleiding van prof. dr. Geert-Jan Kroes in dezelfde Theoretische Chemiegroep. Dat onderzoek resulteerde in het proefschrift wat u hier nu leest. Tijdens deze promotie heeft hij in 2022 meegedaan aan de Han-Sur-Lesse winterschool voor theorie en spectroscopie in Han-Sur-Lesse, België. Ook heeft hij op 20 april 2023 de cursus ‘scientific conduct’ afgerond bij de ‘Graduate School of Science’. Ook was Robert plenaire spreker bij het 2023 HRSMC symposium in Leiden en heeft hij wetenschappelijke posters gepresenteerd op o.a. het CHAINS congres van 2022 in Veldhoven, het HRSMC symposium van 2022 in Amsterdam, en op de Faraday Discussions over ‘New Directions in Molecular Scattering’ van 2024 in Edinburgh, VK. Daarnaast heeft hij ook deelgenomen aan de “High Dimensional Quantum Dynamics” conferentie en workshop van 2022 in Groningen en de N3C conferentie van 2022 in Noordwijkerhout. Na het promotieonderzoek is Robert per 1 juni 2025 verder gegaan bij de Luchtverkeersleiding Nederland (LVNL) als Product Engineer.

Robert A. B. van Bree was born on the 25th of June 1997 in Haarlem, the Netherlands. He graduated high school (VWO) on the 11th of June 2015 at the Rijnlands Lyceum Oegstgeest in Oegstgeest. In the same year he started his Bachelor of Science Molecular Science and Technology a joint degree program between Leiden University and the TU Delft. During his BSc. he wrote his BSc. thesis in experimental surface science under the supervision of Dr. Ludo B. F. Juurlink and Dr. Sabine V. Auras in the group of Catalysis and Surface Chemistry at Leiden University, and he received his *Cum Laude* degree on the 31st of July 2018. Thereafter, he immediately started his Masters of Science Chemistry degree at Leiden University. In his MSc. program he wrote a literature research report regarding the electrolysis of seawater under the supervision of Prof. Dr. Marc T. M. Koper, also at the Catalysis and Surface Chemistry group. Additionally, he wrote his MSc. thesis regarding the fitting of analytical EAM models for Cu(111) under the supervision of Dr. Mark F. Somers and Dr. Bauke Smits at the Theoretical Chemistry group at Leiden University. He received his *Cum Laude* MSc. degree on the 30th of October 2020. Quickly thereafter, on the 1st of November he started his work as a PhD Student under supervision of Prof. Dr. Geert-Jan Kroes in the same Theoretical Chemistry group. This work has resulted in the thesis that you are reading right now. During his PhD he has also attended the 2022 edition of the Han-Sur-Lesse winter school for theory and spectroscopy in Han-Sur-Lesse, Belgium. On the 20th of April 2023 he completed a course on ‘scientific conduct’ at the ‘Graduate School of Science’. Robert was a plenary speaker at the 2023 HRSMC symposium in Leiden and has presented several scientific posters at events including, but not limited to: CHAINS 2022 at Veldhoven, the HRSMC symposium of 2022 in Amsterdam, and the Faraday Discussions on ‘New Directions in Molecular Scattering’ in 2024, Edinburgh, UK. Lastly, he also took part in the “High Dimensional Quantum Dynamics” conference and workshop of 2022 in Groningen and the N3C conference of 2022 in Noordwijkerhout. After his PhD Robert has started work at Luchtverkeersleiding Nederland (LVNL) as a Product Engineer on June 1st 2025.

List of publications

- van Bree, R. A. B.; Kroes, G. J. Limits of BOSS DFT: O₂ + Al(111) Dynamics on a Screened Hybrid Van der Waals DFT Potential Energy Surface. *J. Phys. Chem. C* **2025**, *129* (11), 5408–5421.
<https://doi.org/10.1021/acs.jpcc.5c00327>.
- van Bree, R. A. B.; Kroes, G. J. O₂ Dissociation on Cu(111) Dynamics on a Novel Screened Hybrid Van der Waals DFT Potential Energy Surface. *J. Phys. Chem. C* **2024**, *128* (45), 19182–19196.
<https://doi.org/10.1021/acs.jpcc.4c05466>.
- van Bree, R. A. B.; Gerrits, N.; Kroes, G.-J. Dissociative Chemisorption of O₂ on Al(111): Dynamics on a Potential Energy Surface Computed with a Non-Self-Consistent Screened Hybrid Density Functional Approach. *Faraday Discuss.* **2024**, *251*, 361–381.
<https://doi.org/10.1039/D3FD00165B>.
- Auras, S. V.; van Bree, R. A. B.; Bashlakov, D. L.; van Lent, R.; Juurlink, L. B. F. It's Not Just the Defects – a Curved Crystal Study of H₂O Desorption from Ag. *Phys. Chem. Chem. Phys.* **2019**, *21* (28), 15422–15430.
<https://doi.org/10.1039/C9CP02609F>.

Afterword

In writing these word I am writing what will be the final words of this thesis, and some of the last blank pages that needed to be overcome. The last four and half years have been far from easy, starting a PhD in a time that turned out to be the height of a global pandemic was a demanding task. Thereafter, as some things have gotten better whilst others may have gotten worse, both work and life has continued. As such, this thesis is now being wrapped up, both from the author's and the reader's perspective, but before it does end I would like to (at risk of maybe forgetting some people) say my thanks.

First and foremost, I thank my promoters Prof. Dr. Geert-Jan Kroes and Dr. Jörg Meyer without whom this thesis could never have existed, nor would I have learned to write, analyse and practice science as I now do.

I wish also to thank Dr. Mark Somers, who started out as my mentor during my MSc. in the TC-group and has never let that role go when I moved on to doing a PhD. Neither would my knowledge of HPC, computers, programming, systematism in work, beers, bars, and hiking be what it is without his enthusiasm, guidance and assistance.

Furthermore, I would like to thank all the students who have worked on my many small, preliminary, research projects which were instrumental in showing us the things we should do or more often the things we should *not* do. These students include but are not limited to my BSc. student Floris Löffler, and MSc. students Laura Viaud and Sanne Starmans

I would also like to thank Bauke Smits for first supervising my MSc. degree and then welcoming me as a valued colleague. Additionally, I thank Joan Enrique Romero, Theophile Tchakoua, Lukas Hückmann, Jonathon Cottom, Floris van den Bosch, Brian Ferrari, and Nick Gerrits for the fun and insightful discussions on all things (surface) science. I would also like to thank Carson Mize, with whom the discussions were often more joyful and ridiculous than necessarily insightful. And of course I also thank: Guido Smeets, Paul Spiering, Justina Moss, Thanja

Lamberts, Marten Raaphorst, Darío Barreiro Lage, and the rest of the TC group for the amazing years working among them.

Additionally, I would also like to thank Koen, Laurens, Quintijn, Sjoerd, Ischa, Frair, Teunis, Jasper, Marijn and many more friends who have been with me through the good and the bad times of not just this PhD.

Last but absolutely not least, I would like to greatly thank my family: Carla, Joost, and Mathijs who have always been there for me.