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Accurate modeling of the dynamics of dissociative chemisorption on metal surfaces

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Curriculum Vitae

Nick Gerrits is geboren op 8 juli 1992 te Dordrecht. In 2010 heeft hij zijn gymnasiumdiploma *cum laude* behaald aan het Johan de Witt-gymnasium in Dordrecht. In hetzelfde jaar is hij begonnen aan de bacheloropleiding “Molecular Science and Technology” aan de Universiteit Leiden en de Technische Universiteit Delft. Na het behalen van zijn bachelordiploma in 2015 is hij begonnen aan de masteropleiding “Chemistry”, tevens aan de Universiteit Leiden. Als onderdeel van deze opleiding heeft hij onderzoek gedaan onder begeleiding van dr. Jörg Meyer in de Theoretische Chemie groep in Leiden, en heeft hij een Erasmus stage gedaan bij de Centro de Física de Materiales in San Sebastian, Spanje, onder begeleiding van dr. Iñaki Juaristi. Dit onderzoek was gericht op het berekenen van elektronischefrictiecoëfficiënten met behulp van verschillende benaderingen. Tijdens zijn bachelor- en masteropleiding is hij actief geweest bij de studievereniging “Chemisch Dispuut Leiden”, met als hoogtepunten het zijn van de secretaris van het bestuur en de voorzitter van de lustrumcommissie. Na het behalen van zijn masterdiploma in 2017 is hij begonnen met zijn promotieonderzoek onder begeleiding van prof. dr. Geert-Jan Kroes, wederom in de Theoretische Chemie groep in Leiden. Dit heeft geleid tot het proefschrift dat voor u ligt. Vanaf augustus 2021 zal Nick postdoctoraal onderzoek doen in Antwerpen, België, in de PLASMANT groep van prof. dr. Bogaerts, financieel gesteund door een Rubicon beurs van de Nederlandse Organisatie voor Wetenschappelijk Onderzoek. Hier zal hij fundamentele aspecten van plasmakatalyse op metalen oppervlakken onderzoeken.

Nick Gerrits is born on July 8th 1992 in Dordrecht. In 2010 he obtained his gymnasium diploma *cum laude* at the Johan de Witt-gymnasium in Dordrecht. In the same year he started the bachelor study “Molecular Science and Technology” at the Leiden University and the Technical University of Delft. After obtaining his bachelor’s degree in 2015, he started his master study “Chemistry”, also at the Leiden University. As part of this study he performed research under the supervision of Dr. Jörg Meyer in the Theoretical Chemistry group in Leiden, and he performed an Erasmus research internship

at the Centro de Física de Materiales in San Sebastian, Spain, under the supervision of Dr. Iñaki Juaristi. This research was aimed at calculating electronic friction coefficients using several approximations. During his bachelor and master studies he has been active at the study association “Chemisch Dispuut Leiden”, with highlights being the secretary of board and the president of the lustrum committee. After obtaining his master’s degree in 2017, he started his PhD research under supervision of Prof. Dr. Geert-Jan Kroes, again in the Theoretical Chemistry group in Leiden. This has led to the thesis in front of you. From August 2021 onward, Nick will perform postdoctoral research in Antwerp, Belgium, in the PLASMANT group of Prof. Dr. Bogaerts, financially supported by a Rubicon grant from the Dutch Research Council. Here, he will investigate fundamental aspects of plasma catalysis on metal surfaces.

List of Publications

- Gerrits, N.; Migliorini, D.; Kroes, G.-J. Dissociation of CHD₃ on Cu(111), Cu(211), and Single Atom Alloys of Cu(111). *J. Chem. Phys.* **2018**, *149*, 224701, DOI: [10.1063/1.5053990](https://doi.org/10.1063/1.5053990)
- Gerrits, N.; Shakouri, K.; Behler, J.; Kroes, G.-J. Accurate Probabilities for Highly Activated Reaction of Polyatomic Molecules on Surfaces Using a High-Dimensional Neural Network Potential: CHD₃ + Cu(111). *J. Phys. Chem. Lett.* **2019**, *10*, 1763–1768, DOI: [10.1021/acs.jpcllett.9b00560](https://doi.org/10.1021/acs.jpcllett.9b00560)
- Gerrits, N.; Kroes, G.-J. An AIMD Study of Dissociative Chemisorption of Methanol on Cu(111) with Implications for Formaldehyde Formation. *J. Chem. Phys.* **2019**, *150*, 024706, DOI: [10.1063/1.5070129](https://doi.org/10.1063/1.5070129)
- Gerrits, N.; Kroes, G.-J. Curious Mechanism of the Dissociative Chemisorption of Ammonia on Ru(0001). *J. Phys. Chem. C* **2019**, *123*, 28291–28300, DOI: [10.1021/acs.jpcc.9b09121](https://doi.org/10.1021/acs.jpcc.9b09121)
- Gerrits, N.; Chadwick, H.; Kroes, G.-J. Dynamical Study of the Dissociative Chemisorption of CHD₃ on Pd(111). *J. Phys. Chem. C* **2019**, *123*, 24013–24023, DOI: [10.1021/acs.jpcc.9b05757](https://doi.org/10.1021/acs.jpcc.9b05757)
- Gerrits, N.; Geweke, J.; Smeets, E. W. F.; Voss, J.; Wodtke, A. M.; Kroes, G.-J. Closing the Gap Between Experiment and Theory: Reactive Scattering of HCl from Au(111). *J. Phys. Chem. C* **2020**, *124*, 15944–15960, DOI: [10.1021/acs.jpcc.0c03756](https://doi.org/10.1021/acs.jpcc.0c03756)
- Gerrits, N.; Juaristi, J. I.; Meyer, J. Electronic Friction Coefficients from the Atom-in-Jellium Model for $Z = 1 - 92$. *Phys. Rev. B* **2020**, *102*, 155130, DOI: [10.1103/PhysRevB.102.155130](https://doi.org/10.1103/PhysRevB.102.155130)
- Gerrits, N.; Smeets, E. W. F.; Vuckovic, S.; Powell, A. D.; Doblhoff-Dier, K.; Kroes, G.-J. Density Functional Theory for Molecule–Metal Surface Reactions: When Does the Generalized Gradient Approximation Get It Right, and What to Do If It Does Not. *J. Phys. Chem. Lett.* **2020**, *11*, 10552–10560, DOI: [10.1021/acs.jpcllett.0c02452](https://doi.org/10.1021/acs.jpcllett.0c02452)

- Gerrits, N.; Geweke, J.; Auerbach, D. J.; Beck, R. D.; Kroes, G.-J. Highly Efficient Activation of HCl Dissociation on Au(111) via Rotational Pre-excitation. *J. Phys. Chem. Lett.* **2021**, *12*, 7252–7260, DOI: [10.1021/acs.jpcllett.1c02093](https://doi.org/10.1021/acs.jpcllett.1c02093)

Afterword

Having completed my PhD thesis, I would like to thank many people that have been involved in some way or another. Since I am thankful to so many people, I am extremely sorry if I forgot to mention you. After these apocalyptic four years (e.g., Trump, Brexit, corona, Rutte's memory, and the ever increasing prices on beer), it is easy to forget.

First and foremost, I would like to thank my supervisor Geert-Jan Kroes. This thesis would not have been possible without your help and guidance. You always managed to push me to achieve more and to provide me with insights into the wonderful world of academia. Additionally, you afforded me an enormous amount of freedom in my research. Although this led to a thesis that might not resemble at all what we initially set out to do, I think we can be even happier with the end result.

I wish to thank Jörg Meyer for guiding me into the world of computational surface science during my master. You provided me with the tools to start my journey into research.

I am grateful to Mark Somers for teaching me how to approach computing and providing me with different views on university matters. While I do not share your very clear preference of La Chouffe and I think it is better in the future to avoid pitchers filled with Grimbergen Tripel, the beer-infused discussions at the Foobar were very enjoyable.

I am thankful to Thanja Lamberts for helping me to discover the next step in my career and being available for coffee or lunch during the very lonely corona office days. You always reminded me to be open minded. Also, it was funny to see such a positive person being so great at complaining about stuff.

Marc van Hemert, it was always very enjoyable to hear stories from times long past and your view on what a good scientist is supposed to be.

I thank Davide Migliorini, Helen Chadwick, and Francesco Nattino for teaching me how to do AIMD simulations on methane reactions, as this was the start of all the work forming this thesis. Without you the AIMD dance would not have existed.

I am happy that I could share some of the things I have learned during my PhD with my students Jeffrey Talboom and Sanne Starmans. I would also like

to give a honorable mention to my LO-students Felix Hall and Steven Jansen for a beautiful (meme) pie of me.

I am particularly grateful to Guido Smeets and Paul Spiering for being there during my master and PhD. You knew how to appreciate and contribute to the endless stream of jokes in the office, during breaks and, perhaps most importantly, while having drinks. With the discussions on work and matters concerning life in general combined with helping each other out with issues, I am certain our office was much better for it, despite perhaps not being the "quiet" office.

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Although not as often as during my bachelor or master's studies, I have enjoyed many of the "extracurricular" activities with the Chemisch Dispuut Leiden and the Brouwmeesters.

I am happy to have so many friends that have supported me in some way these years. Whether we mowed the grass at a hardstyle festival, tasted (not so) excellent beer, dissected the weirdest movies, fired up the BBQ irrespective of the weather, or simply had a good time together, you helped me to stay energetic. Thanks to all of you.

Special thanks to my parents and grandparents, and Dionne's parents for their support.

Finally, I especially thank Dionne. We met when I started my PhD and you have been a constant in my life ever since.