Surface temperature and the dynamics of H2 on Cu(111)

Smits, B.

Curriculum vitae

Bauke Smits is geboren op 2 februari 1994 te Zuidland. In 2012 heeft hij zijn gymnasiumdiploma behaald aan het Penta college Blaise Pascal te Spijkenisse.In ditzelfde jaar begon hij de bacheloropleiding "Molecular Science and Technology" aan de Universiteit Leiden en de Technische Universiteit Delft. Deze opleiding rondde hij af in 2015 met een onderzoeksproject onder begeleiding van dr. Mark Somers binnen de Theoretische Chemie groep van het "Leiden Institute of Chemistry", onderdeel van Leiden University. Hierbij is de invloed van de afkapafstand binnen het statische corrugatie model bestudeerd. Vervolgens ging hij verder met de masteropleiding "Chemistry" aan de Universiteit Leiden, waar hij onder begeleiding van dr. Hugo van Ingen zwakke koppeling tussen magnetisch inequivalente rotaties onderzocht. Na het behalen van zijn masterdiploma in 2018, startte hij met zijn promotieonderzoek onder de promotor prof.dr. Geert-Jan Kroes met directe begeleiding van co-promotor dr. Mark Somers, wat uiteindelijk leidde tot dit proefschrift. Vanaf april 2023 zet hij zijn onderzoek naar temperatuurseffecten op de waterstof op koperreactie voort met een vervolgonderzoek onder begeleiding van dr. Jörg Meyer and dr. Mark Somers.

List of publications

- Wijzenbroek, M.; Klein, D. M.; Smits, B.; Somers, M. F.; Kroes, G.-J. Performance of a Non-Local van der Waals Density Functional on the Dissociation of H $_2$ on Metal Surfaces. *The Journal of Physical Chemistry A* **2015**, *119*, 12146–12158, DOI: 10.1021/acs.jpca.5b06008

- le Paige, U. B.; Smits, B.; 't Hart, P.; Lefeber, F.; Martin, N. I.; van Ingen, H. Weak Coupling between Magnetically Inequivalent Spins: The Deceptively Simple, Complicated Spectrum of a 13C-labeled Trimethylated Amine. *Journal of Magnetic Resonance* **2017**, *278*, 96–103, DOI: 10.1016/j.jmr.2017.03.016

- Smits, B.; Somers, M. F. Beyond the static corrugation model: Dynamic surfaces with the embedded atom method. *The Journal of Chemical Physics* **2021**, *154*, 074710, DOI: 10.1063/5.0036611

- Smits, B.; Litjens, L. G. B.; Somers, M. F. Accurate Description of the Quantum Dynamical Surface Temperature Effects on the Dissociative Chemisorption of H_2 from Cu(111). *The Journal of Chemical Physics* **2022**, *156*, 214706, DOI: 10.1063/5.0094985

- Smits, B.; Somers, M. F. The Quantum Dynamics of H_2 on Cu(111) at a Surface Temperature of 925 K: Comparing State-of-the-Art Theory to State-of-the-Art Experiments. *The Journal of Chemical Physics* **2022**, *157*, 134704, DOI: 10.1063/5.0112036

- Smits, B.; Somers, M. F. The Quantum Dynamics of H_2 on Cu(111) at a Surface Temperature of 925 K: Comparing State-of-the-Art Theory to State-of-the-Art Experiments 2. *The Journal of Chemical Physics* **2023**, *158*, 014704, DOI: 10.1063/5.0134817

Afterword

With this I now write the final parts of this thesis, which was most of all dominated by what the Dutch liked to call "lastige tijden". Nevertheless with some delay it formed into a full story about one very specific effect for one very specific system, which hopefully will at some point see an expansion to more general use. With the major risk of forgetting a lot of people, I will still try to at least say my thanks.

First of all, of course, to Mark Somers who snagged me from my Master's defence into this project. You provided the basis of this project with a clear goal and path to get there, yet left enough open for me to pursue my own approaches. Furthermore, under your guidance I got to learn the basics of both managing our HPC hardware and finding the best bars.

I am grateful for the scientific support and guidance of my promotor Geert-Jan Kroes. My thanks also to my desk-neighbour Marc van Hemert, who could always supply another point of view to any encountered problem, as well as Jörg Meyer, who has given me the opportunity to continue working on this system just a little longer.

Thanks also go out to Leandra Litjens and Ruard van Workum, the bachelor students I had the pleasure to supervise during this project. Not to be forgotten is then of course my only master student, and now colleague, Robert van Bree. Your master's project was a bit of a rocky journey, but that has never stopped you complaining about especially the little things.

I would be amiss to not also thank the PhD students who showed me the ropes: Paul Spiering, Guido Smeets, and Nick Gerrits. My thanks also go to Theophile Tchakoua, the fellow PhD student who might have started slightly before me, but taught me all about both unique types of food and paying at bars.

A further thanks for the people who are part of theoretical chemistry now, or in the past, who made the coffee breaks a lively place: Lukas Hückmann, Brian Ferrari, Floris van den Bosch, Marten Raaphorst, Tim Jansen, Justina Moss, Joan Enrique Romero, Jonathon Cottom, Andrew Powell, Seenivasan Hariharan, Khosrow Shakouri, Helen Chadwick, Katharina Doblhoff-Dier, Thanja Lamberts, Michelle van der Haar, Soroush Rasti, Sayan Seal, Hossein Tahmasbi, and Elham Nour Ghassemi.

Thanks to the boys from the Blaise Pascal, Floyd, Pepijn, Robert, and Laurens, we might have taken different routes in life but there will always be something that connects us. A thank you to my British friend "Pepi", for our love for a very specific news broadcast. And of course a thank you to Desiree, who allows me to try out many of the co-op games I find.

Finally, as always, the biggest of thanks to my family and grandparents, who would always try to understand my work, even if I myself didn't.