



Universiteit
Leiden
The Netherlands

Hydrogen dissociation on metal surfaces: A semi-empirical approach

Nour Ghassemi, E.

Citation

Nour Ghassemi, E. (2019, September 19). *Hydrogen dissociation on metal surfaces: A semi-empirical approach*. Retrieved from <https://hdl.handle.net/1887/76855>

Version: Not Applicable (or Unknown)

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

Downloaded from: <https://hdl.handle.net/1887/76855>

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

Cover Page



Universiteit Leiden



The following handle holds various files of this Leiden University dissertation:
<http://hdl.handle.net/1887/76855>

Author: Nour Ghassemi, E.

Title: Hydrogen dissociation on metal surfaces: A semi-empirical approach

Issue Date: 2019-09-19

Curriculum Vitae

Elham Nour Ghassemi was born on March, 21 1980 in Tabriz (Iran). In 1999, she was graduated in Mathematics and Physics from Tohid high school, Tabriz, Iran. She received her BSc degree in Solid State Physics from Azerbaijan University, Tabriz, Iran. After receiving her bachelor's degree in 2003, she studied Solid State Physics and Electronics at the University of Tabriz from 2003 to 2005, obtaining her master degree. She started working at the lab located in Isfahan University of Technology, as a teacher and research assistance for three years. On September 2008, she moved to Stockholm, Sweden, where she got admitted to work as a research assistance at Stockholm University under supervision of Prof. dr. Åsa Larson and Dr. Jonas Larson in the faculty of science in theoretical physics and the molecular physics department. She received a second master degree in 2011 and continued her collaboration with Stockholm University until 2012. On January 2014, she joined the group of Prof. dr. Geert-Jan Kroes at the Leiden Institute of Chemistry of Leiden University, The Netherlands as a PhD candidate. Her research was funded by an ERC Advanced grant. Her research led to a number of publications and this thesis.

List of Publications

1. J. Larson, E. Nour Ghassemi and Å. Larson "Anomalous Molecular Dynamics in the Vicinity of a Conical Intersection" *EPL (Europhysics Letters)* 101, 43001 (2013).
2. E. Nour Ghassemi, J. Larson, Å. Larson, "A Diabatic Representation of the Two Lowest Electronic States of Li_3 " *The Journal of Chemical Physics* 140, 154304 (2014).
3. E. Nour Ghassemi, M. Wijzenbroek, M. F. Somers, and G. J. Kroes, "Chemically Accurate Simulation of Dissociative Chemisorption of D_2 on Pt(111)" *Chemical Physics Letters*, 683, 329-335 (2017).
4. E. Nour Ghassemi, M. F. Somers and G. J. Kroes, "Test of the Transferability of the Specific Reaction Parameter Functional for $\text{H}_2 + \text{Cu}(111)$ to $\text{D}_2 + \text{Ag}(111)$ " *The Journal of Physical Chemistry C*, 122, 22939-22952 (2018).
5. E. Nour Ghassemi, E. W. F. Smeets, M. F. Somers, G. J. Kroes, I. M. N. Groot, L. B. F. Juurlink, G. Fuchs, "Transferability of the Specific Reaction Parameter Density Functional for $\text{H}_2 + \text{Pt}(111)$ to $\text{H}_2 + \text{Pt}(211)$ " *The Journal of Physical Chemistry C* 123(5), 2973-2986 (2019).
6. E. Nour Ghassemi, M. F. Somers, and G. J. Kroes, "Assessment of Two Problems of Specific Reaction Parameter Density Functional Theory: Sticking and Diffraction of H_2 on Pt(111)" *The Journal of Physical Chemistry C* 123(16), 10406-10418 (2019).

Afterword

On January 2014, when I started my journey as a “ *PhD candidate* ”, to me, it seemed like a magic to finish it. Now the journey is about to finish and the magic is going to happen. I owe this to my kind and supportive supervisors, colleagues, friends and family members. This work would not have been possible without the valuable assistance of them. Here, I would like to devote this space to thanking those who have walked alongside me during this journey and made the magic happen.

To *Geert-Jan Kroes* : thanks for providing me this wonderful opportunity of being a member of the LIC family. I learned, grew and enjoyed every moment of working there.

It is my greatest duty to express my deep regards and gratitude to *Mark Somers*, for under whose guidance and supervision I was able to undertake this project.

I am also grateful to the European Research Council (ERC), who funded this work.

To my committee members, *Prof. dr. H. S. Overkleeft*, *Prof. dr. M. T. M. Koper*, *Prof. dr. H. J. M. de Groot*, *Prof. dr. A. Groß*, *Prof. dr. G. C. Groenenboom*, *Dr. C. Díaz*, and *Dr. I. M. N. Groot*: I am appreciative of you for evaluating my thesis and be a member of my graduation committee.

To my project teammates, *Gernot Füchsel*, *Irene Groot*, *Ludo Juurlink*, *Egidius Smeets* and *Mark Wijzenbroek*: I am so grateful for the support and assistance provided by you. Thank you for all the generous advises. Discussing with you about the challenges has been always constructive and valuable to me. This thesis truly is the result of all those daily discussions.

To my creative and smart colleagues, *Davide Migliorini*, *Khosroe Shakori*, *Francesco Nattino*, *Katharina Doblhoff-Dier*, *Paul Spiering*, *Nick Gerrits*, *Jörg Meyer*, *Sayan Seal*, *Soroush Rasti*, *Theophile Tchakoua*, *Andrew Powell*, *Francesca Costanzo* and *Marc van Hemert* : I am indebted to you all. I

enjoyed every moment that we spent together. I will never forget all those small chats, coffee breaks, Friday talks.

To *Michelle van der Haar*: I am truly appreciated by the assistance provided by you. You have been always there to help me with all the steps that could accelerate required official procedures.

To my master supervisors in Stockholm University, *Asa Larson* and *Jonas Larson*, I would like to thank you for your kind supports and encouragements.

To my truly friends, *Soodeh*, and *Leila*, you have been always like a sister to me. You and your lovely families have been always there to lend me and my family a hand without hesitate. Me and my family will never forget your assistance and support.

To my kind friends, *Faezeh*, *Fatemeh*, *Afsaneh*, *Gerrie*, *Hanieh*, *Sara*, and other my *Gezellig* friends, thank you for all the warm and friendly gatherings.

To my dance teacher, *Sofya*, I released all my tiredness after hard working in your excellent Salsation classes and boosted my energy to do the best for the next day.

To my piano teacher, *Maria*, thank you for your encouraging word during the period that I had been writing my thesis and for our great chats.

To my kind in-laws, *Simin*, *Reza*, *Noushin* and *Farrin*: I owe a deep gratitude and thanks for your positive attitude and encouragement in all the steps.

To my incredible parents, *Farahnaz* and *Jalil*: I cannot express anything that can show my gratefulness for your love and encouragement. You are always ready to provide me hope and motivation for my next step. I would never have enjoyed so many wonderful opportunities without your endless sacrifice.

To my brother, *Behnam*: I am more than grateful to you. You were always kindly supporting my decisions. I hope I can spend more time later with you and your beloved families: *Loyan*, and *Sara*.

I save the last for the best. To my **lifelong friend**, *Afshin*: this would not be achieved without your support and patience. During this journey you have been always passionate, empathetic, persistent and considerate.

Finally I take pride in dedicating the current PhD thesis work to my **beloved son**, *Radin*. I love you for everything, for being so understanding through the toughest moments of my life. I hope be a good mom and spend more time with you.