From models to mechanisms: defects and charge trapping in amorphous silicon nitride

Hückmann, L.

Publications

Journal Publications

[1] **Hückmann, L.**; Cottom, J.; Meyer, J. "Intrinsic Charge Trapping and Reversible Charge Induced Structural Modifications in a-Si_3N_4" *Adv. Phys. Res.* **2024**, *3*, 2300109.

[2] Cottom, J.; **Hückmann, L.**; Olsson, E.; Meyer, J. "From Jekyll to Hyde and Beyond: Hydrogen's Multifaceted Role in Passivation, H-Induced Breakdown, and Charging of Amorphous Silicon Nitride" *J. Phys. Chem. Lett.* **2024**, *15*, 840–848. *Selected for cover.*

[3] Cottom, J.; **Hückmann, L.**; Meyer, J.; Olsson, E. "Forged by Charge: Polaron-Induced Matrix Formation in Silicon Nitride Conversion-Type Anodes for Lithium-ion Batteries" *J. Mater. Chem. A* **2025**, *13*, 34260–34272. *HOT paper, selected for cover.*

[4] **Hückmann, L.**; Sylvia, R.; Blankenvoorde, F.; Cottom, J.; Meyer, J. "Mechanistic Insights into the Dry Oxidation of Amorphous Silicon Nitride: A DFT Study" *J. Mater. Chem. C* **2026**, *14*, 139–151. *Selected for cover.*

[5] **Hückmann, L.**; Sanders, M.; Cottom, J.; Meyer, J. "Application-Tailored Classical Interaction Potentials: A Workflow Based on Bayesian Optimization" **2026**, *in preparation.*

Journal Publications (not included)

[6] **Hückmann, L.**; Cottom, J.; Meyer, J.; Olsson, E. "Topology-Directed Silicide Formation: An Explanation for the Growth of C49-$TiSi_2$ on the Si(100) Surface" *arXiv* **2026**. DOI: 10.48550/arXiv.2601.10368

Open Science

I made several contributions related to the publications this thesis was based on in the form of publicly released source code:

Source code

- The source code used to determine the opening angles in coordination polyhedra from Section 3.1.3:
  `https://github.com/lhuckmann/cone_analysis_tool.git`
- The source code for the Bayesian Optimization Force Field fitting scheme presented in Chapter 4 is available under:
  `https://github.com/lhuckmann/BOFFfit.git`

Data availability

- The a-Si_3N_4 structure library and simulation scripts from Chapter 5 are available under `https://doi.org/10.5281/zenodo.18887677`
- The a-Si_3N_4:H structure library from Chapter 6 is available under
  `https://doi.org/10.5281/zenodo.10054617`
- The a-Si_3N_4:O structure library from Chapter 7 is available under
  `https://doi.org/10.5281/zenodo.15206130`
- The a-Si_3N_4:Li structure library from Chapter 8 is available under
  `https://doi.org/10.5281/zenodo.15297234`

Afterword

It goes without saying that this thesis could not have been written without the support of many remarkable people to whom I owe my deepest gratitude.

First and foremost, I would like to thank **Jörg Meyer** for welcoming me into his group, for his guidance, and for supporting my development in every conceivable way. His scientific insight, encouragement, and trust have been indispensable throughout this journey.

I am equally grateful to **Jonathon Cottom**, who has been my mentor over these years. His influence extends far beyond scientific matters: He sharpened my awareness of the broader meaning and responsibility of research, continually challenged my thinking, and encouraged me to reflect critically on both my work and myself.

Special thanks are also owed to **Emilia Olsson**, who welcomed me as a guest researcher in her group at the Advanced Research Center for Nanolithography (ARCNL) from September 2024 onward. Through our collaboration, I had the invaluable opportunity to gain firsthand experience with the complex phenomena that govern surfaces and interfaces.

My sincere thanks also go to the entire Theoretical Chemistry Group at Leiden University. In particular, I thank **Mark Somers** for keeping our computers running, and **Robert van Bree**, **Bauke Smits**, **Theophile Tchakoua**, and **Justina Moss** for making me feel immediately at home upon arriving in the Netherlands. Special thanks also to **Carson Mize**, who became a dear friend to me during this time. Many thanks as well to **Bibiana Türkcan** for her help with the Dutch translation and **Tobias Dijkhuis**, whose Blender scripts were put to good use in this thesis. I would also like to acknowledge **Emma Carels**, **Floris van den Bosch**, **Brian Ferrari**, **Nick Gerrits**, **Marten Raaphorst**, **Joan Enrique-Romero**, **Darío Barreiro Lage**, **Neven Golenić**, **Younes Akabli**, **Geert-Jan Kroes**, **Thanja Lamberts**, and **Katharina Doblhoff-Dier** for creating a stimulating and friendly environment, and one that

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I would also like to express my gratitude to the Materials Theory and Modeling Group at ARCNL for their warm welcome and for making my time there a pleasant and enriching experience. Thus, I wish to acknowledge **Barsha Bhattacharjee**, **Robin Delhomme**, **Thomas Nieboer**, **Giona Mainardis**, and **Gabrielli Almeida**.

But all of that would not have been possible without several important people in the background. That is why I also want to acknowledge my teachers at the University of Stuttgart, first and foremost **Johannes Kästner**, who paved the way for my journey, which cannot be stressed enough. Likewise, I would like to thank all the wonderful friends and family members who encouraged me throughout this adventure and were part of this journey. In particular, I thank my fellows from Stuttgart **Kim** and **Julian Mehnert-Birk**, **Alexander Waigum**, **Patrick Probst**, and **Sofia Kolin** as well as my parents, **Jochen** and **Helma**, and my sisters, **Anne** and **Jule**. And last, I thank **Carolin Rieg**, for her support and for being by my side throughout this long journey.

Without you all, this would not have been possible.

Curriculum vitae

Lukas Hückmann was born on March 23rd 1996 in Mühlacker, Baden-Württemberg, Germany. He obtained his Abitur from the Alfred-Amann-Gymnasium in 2014 and subsequently enrolled at the University of Stuttgart to pursue a Bachelor of Science in Mathematics. After changing his field of study to Chemistry in the winter semester of 2015, he completed his Bachelor's degree in 2020 with a thesis in theoretical chemistry entitled *Study of the Ruthenium-Catalyzed Alkylation of Aniline*, carried out in the group of Johannes Kästner. He continued his studies at the University of Stuttgart and received his Master of Science in Chemistry in 2022, working under the supervision of Viktor Zaverkin in the Kästner group on *Construction of Accurate and Efficient Water Models via Machine Learning*.

He subsequently began his Ph.D. at Leiden University in the Theoretical Chemistry Group led by Jörg Meyer. During this time, he attended the Han-sur-Lesse Winter School for Theoretical Chemistry and Spectroscopy in 2022, 2023, and 2024, as well as courses on *Scientific Conduct* and the Wiley workshop *Writing Your Scientific Paper*. He delivered oral presentations of his research at the NWO CHAINS conference 2023 in The Hague, the NWO Physics conference 2025 in Veldhoven, the 17th International Conference on Materials Chemistry (MC17) in 2025 organized by the Royal Society of Chemistry in Edinburgh, and at the HRSMC Symposium 2025 in Amsterdam.

From September 2024 onward, he joined the Advanced Research Center for Nanolithography (ARCNL) as a guest researcher in the Materials Theory and Modeling group led by Dr. Emilia Olsson, extending his research to the study of surfaces and interface formation in silicon-based materials. In the near future, he will continue completing his ongoing projects in the Theoretical Chemistry Group in Leiden before pursuing new opportunities.