

## Dr. Vanessa J. Bukas



### Current Position

Group Leader, Theory Dept. of the FHI, MPG (since 2021)

### Previous Positions/ Education

- Parental leave (2022)
- PostDoc at Catalysis Theory Center | Prof. J. K. Nørskov group  
Physics Dept., Technical Univ. Denmark (2018-2021)
- PostDoc at SUNCAT Center for Interface Science and Catalysis | Prof. J. K. Nørskov group  
Stanford Univ. (2017-2018)
- PhD (summa cum laude) in Theoretical Chemistry | Prof. K. Reuter group  
Chemistry Dept., TU München (2016)
- MSc in Advanced Materials Science (ECTS grade: A “Excellent”) | Elite Network of Bavaria  
program co-organized by LMU München, TU München & Uni. Augsburg (2010-2012)
- Research assistant at the National Hellenic Research Foundation, Athens (2009-2010)
- Diploma in Applied Mathematics & Physics (GPA: 8.2/10)  
National Technical University Athens (2003-2009)

### Research Expertise

Theoretical / computational catalysis, predictive-quality multiscale modeling, heterogeneous thermal & electro-catalysis, energy conversion at interfaces

### Honors/ Awards

- H. C. Ørsted COFUND PostDoc fellowship (2019-2021) | Marie Skłodowska-Curie under EU  
Horizon 2020
- Speaker at the 65th Lindau Nobel Laureate meeting (2015)
- Onassis MSc scholarship (2010-2012) | Alexander S. Onassis Public Benefit Foundation

### Key publications ([ORCID](#), [Google Scholar](#))

- V. J. Bukas, K. Reuter, “[Hot adatom diffusion following oxygen dissociation on Pd\(100\) and Pd\(111\): A first-principles study of the equilibration dynamics of exothermic surface reactions](#)”, *Phys. Rev. Lett.* 117, 14, 146101 (2016)
- V. J. Bukas, H. W. Kim, R. Sengpiel, K. Knudsen, J. Voss, B. D. McCloskey, A. C. Luntz, “[Combining experiment and theory to unravel the mechanism of two-electron oxygen reduction at a selective and active co-catalyst](#)”, *ACS Catal.* 8, 12, 11940-11951 (2018).
- S. Z. Andersen, M. J. Statt, V. J. Bukas, S. G. Shapel, J. B. Pedersen, K. Krempel, M. Saccoccio, D. Chakraborty, J. Kibsgaard, P. C. K. Vesborg, J. K. Nørskov, I. Chorkendorff, “[Increasing stability, efficiency, and fundamental understanding of lithium-mediated electrochemical nitrogen reduction](#)”, *Energy Environ. Sci.* 13, 11, 4291-4300 (2020).
- K. Li, S. Z. Andersen, M. J. Statt, M. Saccoccio, V. J. Bukas, K. Krempel, R. Sažinas, J. B. Pedersen, V. Shadravan, Y. Zhou, D. Chakraborty, J. Kibsgaard, P. C. K. Vesborg, J. K. Nørskov, I. Chorkendorff, “[Enhancement of lithium-mediated ammonia synthesis by addition of oxygen](#)”, *Science* 374, 6575, 1593-1597 (2021).
- A. Cao, V. J. Bukas, V. Shadravan, Z. Wang, H. Li, J. Kibsgaard, I. Chorkendorff, J. K. Nørskov, “[A spin promotion effect in catalytic ammonia synthesis](#)”, *Nat. Commun.* 13, 1, 2382 (2022).
- A. M. Dudzinski, E. Diesen, H. H. Heenen, V. J. Bukas, K. Reuter, “[First step of the Oxygen Reduction Reaction on Au\(111\): A Computational Study of O<sub>2</sub> Adsorption at the Electrified Metal/Water Interface](#)”, *ACS Catal.* 13, 18, 12074-12081 (2023).
- H. H. Heenen, H. S. Pillai, K. Reuter, V. J. Bukas, “[Exploring mesoscopic mass transport effects in electrocatalysis](#)”, *ChemRxiv* (2023).