Coupled electronic and nuclear dynamics at interfaces of artificial photosynthesis devices

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Acknowledgements

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Curriculum vitae

Titus de Haas was born on the 13th of November 1996 in Amsterdam, the Netherlands, where he spent most of his childhood and early adulthood. Titus went to high school between 2009 and 2015 at the Geert Groote College Amsterdam, where he obtained a VWO diploma (pre-university education) with N&T profile (Nature and Technology, emphasis on natural sciences). After graduating, he went on to pursue a chemistry bachelor's degree program hosted between the University of Amsterdam (UvA) and Vrije Universiteit (VU) Amsterdam. He obtained the BSc. degree in 2018, writing a thesis on cobalt catalyzed water oxidation, which he studied with both experimental and theoretical methods. Following the bachelor, Titus pursued a master's degree in molecular sciences, again at the UvA and the VU. For his thesis he conducted DFT-based research on organometallic chemistry under supervision of Prof. Dr. Peter H.M. Budzelaar at the Federico II university of Naples, in Italy.

After the summer of 2020, Titus started as a PhD candidate at the Leiden Institute of Chemistry in Leiden, the Netherlands, where he was supervised by Dr. Francesco Buda and Prof. Dr. Huub J.M. de Groot. His doctoral research focused on photoinduced charge-separation and catalytic processes for solar-to-fuel production. In this context, he employed density functional and semi-empirical methods to simulate the dynamics of molecules, materials and interfaces in both the ground state and excited states.

Titus showcased his work through multiple presentations at national and international conferences during his PhD studies. Highlights include talks at CHAINS (2022), the Kroese-Duijsters symposium (2023 and 2024), and the HRSMC symposium (2024), and posters at IPQC2023 conference in Bratislava, a Gordon Research Conference (2024) in Easton, Massachusetts, USA, and a

CECAM meeting in Varigotti, Italy. He also won the poster award in the section for Physical Chemistry and Spectroscopy at the 2023 HRSMC symposium.

Beyond research, Titus has been actively involved in teaching at various levels, both during his PhD and as a Master student. He mentored three master's and two bachelor's theses, supervised two *Leren Onderzoeken* projects, and served as a teaching assistant for courses on quantum chemistry, classical mechanics, and practical labs on organic chemistry. During his PhD, Titus followed courses on *Academic Writing*, *Scientific Conduct* and on *How to Write an Excellent Research Grant*. In addition, he was an active board member of the LIC73 PhD and Postdoc group in Leiden, where he contributed to community building.

List of Publications

Main author

1) **T. de Haas**, T. de Jong, H.J.M. de Groot, F. Buda. Non-adiabatic surface hopping dynamics of ultra-fast proton coupled electron transfer in catalyst-dye complex for water oxidation. *Manuscript in preparation*.

2) **T. de Haas***, K. Zhu*, J.M. van der Sterre, Y. Luo, G. Mul, F. Buda and A. Huijser. Effects of Nuclear Motion on the Photoinduced Interfacial Charge Transfer Dynamics at a NiO/P1 Photocathode. *J. Phys. Chem. C*. **2025**, *129* (14), 6817-6826 (* contributed equally)

3) C. Lui*, **T. de Haas***, F. Buda, S. Bonnet. Electron-Withdrawing Effects in Cobalt Porphyrin Catalysts Boost Homogeneous Photocatalytic Hydrogen Evolution in Neutral Aqueous Solutions. *ACS Catal.* **2025***, 15* (6), 4681-4697 (* contributed equally)

4) **T. de Haas***, R. Smit*, A. Tebyani, S. Bhattacharyya, K. Watanabe, T. Taniguchi, F. Buda, M. Orrit. Charge Transfer-Induced Weakening of Vibronic Coupling for Single Terrylene Molecules Adsorbed onto Hexagonal Boron Nitride. *J. Phys. Chem. Lett.* **2025**. *16* (1), 349-356 (*contributed equally)

5) **T. de Haas**, D. Calvani, A. Zaaruolo, T. de Jong, J. Rutgers, B. Kreupeling, H.J.M. de Groot, F. Buda. Hybrid-DFT Molecular Dynamics Simulations of Photocatalytic Water Oxidation in a [Ru-bda]-Dye Complex. *J. Phys. Chem. C*. **2024**. *128* (47), 20093-20103

6) **T. de Haas**, H. van Overeem, H.J.M. de Groot, F. Buda. Strategies to Enhance the Rate of Proton-Coupled Electron Transfer Reactions in Dye-Water Oxidation Catalyst Complexes. *ChemPhotoChem.* **2023***, 7* (3)*, e202200274.*

Co-author

1) C. Liu, A. Amati, **T. de Haas**, F. Buda, A.M. Brouwer, S. Bonnet. Electronic Effects in Water-soluble Zn(II) and Sn(IV) Porphyrin Photosensitizers for Homogeneous Photocatalytic Hydrogen Evolution at pH 7.0. *To be submitted*.

2) K. Zhu, A. P. Rodríguez, M. B. Brands, **T. de Haas**, F. Buda, J. N. H. Reek, G. Mul and A. Huijser. Limiting Molecular Twisting: Upgrading a Donor–Acceptor Dye to Drive H_2 Evolution. *Adv. Sci.* **2024**, *11* (40), 2403454.

3) A. Cataffo, **T. de Haas**, C. Ehm, P. H. M. Budzelaar. Between T and Y: Asymmetry in the Interaction of LAu(I) with Bipy and β-Diiminate-like Ligands. *Eur. J. Inorg. Chem*. **2021**, *2021* (4), 314-320.