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## Photoinduced processes in dye-sensitized photoanodes under the spotlight: a multiscale in silico investigation

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# List of Publications

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## *Main Publications in this Thesis:*

1. **Jan Paul Menzel**, Huub J.M. de Groot, Francesco Buda: “Photoinduced Electron Transfer in Donor-Acceptor Complexes: Isotope Effect and Dynamic Symmetry Breaking”, *Journal of Physical Chemistry Letters*, **2019**, *10*, 6504-6511 (**Chapter 3 of this Thesis**)
2. **Jan Paul Menzel**, Anastasios Papadopoulos, Jelena Belić, Huub J.M. de Groot, Lucas Visscher, Francesco Buda: “Photoinduced Electron Injection in a Fully Solvated Dye-Sensitized Photoanode: A Dynamical Semi-Empirical Study”, *Journal of Physical Chemistry C*, **2020**, *124*, 27965-27976 (**Chapter 4 of this Thesis**)
3. **Jan Paul Menzel**, Martijn Kloppenburg, Jelena Belić, Huub J.M. de Groot, Lucas Visscher, Francesco Buda: “Efficient Workflow for the Investigation of the Catalytic Cycle of a Water Oxidation Catalyst: Combining GFN-xTB and Density Functional Theory”, *Journal of Computational Chemistry*, **2021**, *42*, 1885-1894 (**Chapter 5 of this Thesis**)
4. Tijmen M.A. Bakker, **Jan Paul Menzel**, Bas Vreugdenhil, Tessel Bouwens, Simon Mathew, Francesco Buda, Joost N.H. Reek: “Increased Photocurrent by Improving the Donating Properties of the Anchoring Group in P-Type Dye Sensitized Solar Cells”, *to be submitted* (**Part of Chapter 6 of this Thesis**)
5. **Jan Paul Menzel**, Yorrick Boeije, Tijmen M.A. Bakker, Jelena Belić, Huub J.M. de Groot, Lucas Visscher, Joost N.H. Reek, Francesco Buda: “In Silico Optimization of Charge Separating Dyes”, *to be submitted* (**Part of Chapter 6 of this Thesis**)
6. **Jan Paul Menzel**, Justina Moss, Jelena Belić, Huub J.M. de Groot, Lucas Visscher, Francesco Buda, *in preparation* (**Part of Chapter 7 of this Thesis**)

### *Publications not included in this Thesis:*

1. Helen Chadwick, Han Guo, Ana Gutiérrez-González, **Jan Paul Menzel**, Bret Jackson, Rainer D. Beck: “Methane Dissociation on the Steps and Terraces of Pt(211) Resolved by Quantum State and Impact Site”, *Journal of Chemical Physics*, **2018**, *148*, 014701
2. Han Guo, **Jan Paul Menzel**, Bret Jackson: “Quantum Dynamics Studies of the Dissociative Chemisorption of CH<sub>4</sub> on the Steps and Terraces of Ni(211)”, *Journal of Chemical Physics*, **2018**, *149*, 244704
3. Jelena Belić, Bas van Beek, **Jan Paul Menzel**, Francesco Buda, Lucas Visscher: “Systematic Computational Design and Optimization of Light Absorbing Dyes”, *Journal of Physical Chemistry A*, **2020**, *124*, 6380-6388
4. Jelena Belić, Arno Förster, **Jan Paul Menzel**, Francesco Buda, Lucas Visscher: “Automated Assessment of Redox Potentials for Dyes in Dye-Sensitized Photoelectrochemical Cells”, *Phys. Chem. Chem. Phys*, **2022**, *24*, 197-210
5. Michael S. Meijer, **Jan Paul Menzel**, Matthijs Hakkenes, Francesco Buda, Anne Goetz, Roy van Duijn, Maxime A. Siegler, Sylvestre Bonnet, *in preparation*

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# Curriculum Vitae

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Jan Paul Menzel was born on the 31<sup>st</sup> of January 1992 in the federal city of Bonn (Germany), founded by the Romans on the bank of the river Rhine. Jan Paul grew up with his sister and brother in the part of Bonn that lies on the left bank of the river, where he also went to school at the *Carl-von-Ossietzky Gymnasium* from 2002-2011. After obtaining his *Abitur* with specialization in mathematics and chemistry, he decided to pursue a bachelor's degree in chemistry (2011-2014) in Jena, Thuringia, moving 400 km east over the old inner German border. While living there required some cultural adjustments he soon found fellow chemistry students that quickly became friends and had three wonderful years at the town on the Saale river. While Jan Paul imagined how wonderful chemistry could be without having to worry about yield, he first came into contact with theoretical chemistry. After spending a 5-months ERASMUS period at the NTNU (2013) in Trondheim, Norway, he performed his Bachelor Thesis (Detection and Classification of mycobacteria using Lab-on-Chip SERS) under the supervision of Anna Mühlig, Dr. Dana Cialla-May and Prof. Jürgen Popp in 2014.

Following his Bachelor, Jan Paul decided to leave Germany for the Netherlands to pursue a master's degree in physical chemistry (2015-2017). He furthered his interest in theory and computation through several courses, finalizing his studies with his Thesis (Real time Simulations of Photoinduced Charge Transfer in Molecular Complexes) under guidance of Dr. Francesco Buda and Prof. Huub de Groot. During his master he also went to the University of Massachusetts in Amherst, USA for half a year in 2016 to perform simulations on stepped metal surfaces under supervision of Prof. Bret Jackson and Prof. Geert-Jan Kroes. He obtained his master's degree *cum laude* in April of 2017.

Jan Paul then continued his studies of photoinduced processes using computational tools with Dr. Francesco Buda and Prof. Huub de Groot, culminating in this doctoral thesis (2017-2022). During this time, he supervised first year *Biopharmaceutical*

*Science* students at organic synthesis labs, he prepared exercises and taught and supervised second year *Molecular Science and Technology* students in theoretical chemistry exercise classes. He tutored a total of 4 *Leren Onderzoeken* students, 3 HRSMC research internship students and 5 students performing their master thesis research under his supervision.

Jan Paul presented his research work at a variety of national and international conferences with poster presentations at the PPES conference in Pisa (2018), HRSMC symposium (Leiden, 2018), CTC symposium (Amsterdam, 2019), ISTCP (Tromsø, Norway 2019), Reedijk Symposium (Leiden, 2019), Solar to Products Symposium (Eindhoven, 2019), CHAINS (Veldhoven, 2019, 2021), and ISF Conference (Online, 2021). At this conference he won a poster prize. Oral presentations were given at Han-sur-Lesse Winterschool (2018), CHAINS (Veldhoven/online, 2018, 2020), the HRSMC symposium (Amsterdam, 2019), Physics at Veldhoven (online, 2021) and the Dutch Photochemistry Days (2021).

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I also owe gratitude to my promotor **Huub de Groot** for the great opportunity to perform research at his BPOC/SSNMR group in Leiden. Thank you for your great insight, persistence to put everything on a sound scientific basis and support during this time. Thank you also for the many, sometimes enthusiastic but always productive discussions in both science and other subjects.

I would also like to thank **Jelena**, **Tijmen** and **Lucas Visscher** for fruitful collaborations and scientific discussions during our many meetings.

During my time as a PhD candidate, I had the luck to be able to supervise many talented students: **Stan**, **Klaas**, **Anne**, **Martijn**, **Samantha**, **Yorrick**, **Matthijs** and **Justina**, thank you for your hard work and all the best for your future careers in Science, Business and Education!

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