Jan Paul Menzel

Yale University, New Haven CT, USA

Current Position

Postdoctoral Researcher Since 08/2022
Yale University, New Haven (CT), United States of America

Education

PhD in chemistry, cum laude (within best 5%) 06/2017-03/2022
Universiteit Leiden (UL), The Netherlands
Thesis Title Photoinduced Processes in Dye-Sensitized Photoanodes under the Spotlight
Supervisors Dr. Francesco Buda and Prof. Huub de Groot

Master of Science, Research in Chemistry – Energy and Sustainability, **cum laude** 02/2015-04/2017
Universiteit Leiden (UL), The Netherlands
Supervisors Dr. Francesco Buda and Prof. Huub de Groot
Average Grade: 8.79 (Dutch system with 10 best and 5.5 passed)

Bachelor of Science, Chemistry 10/2011-09/2014
Friedrich-Schiller-Universität Jena (FSU Jena), Germany
Supervisors Dr. Dana Cialla-May, Prof. Jürgen Popp
Average Grade: 1.7 (German system with 1.0 best and 4.0 passed)

Norges Teknisk-Naturvitenskapelige Universitet (NTNU), Trondheim, Norway 08/2013-12/2013
Study exchange

Research Experience

Postdoctoral Research – ***Yale University***, *United States of America* Since 08/2022
Supervisor Prof. Victor Batista
Mechanistic studies of photocatalytic fuel production on GaN nanowires using plane wave DFT. Effect of surface defects and surface oxidation on photocatalytic conversion. Effect of doping on band structure of semiconductors. Photoinduced interfacial charge transfer dynamics. Semi-empirical based molecular dynamics in extended systems, including solid-liquid interfaces of several hundred atoms. High throughput screening and data extraction of 100 000s of molecules using semi-empirical methods for training of generative Machine Learning models. Redox studies on transition metal complexes. Electronic structure and charge carrier dynamics in semiconductors.

PhD Research – ***UL***, ***HRSMC***, *The Netherlands* 06/2017-06/2022
Supervisors Dr. Francesco Buda and Prof. Huub de Groot
In silico Design of a Photoanode in a dye-sensitized photoelectrochemical cell. Simulations of photoinduced electron injection in a dye-sensitized photoanode using a combination of SCC-DFTB for nuclear dynamics and the AO/MO propagator and an Extended Hückel Hamiltonian for quantum dynamics of photoexcited electron and hole. Determination of importance of nuclear motion, conformational and trajectory averaging and explicit solvation. Evaluation of electron injection performance of several anchoring groups and dyes. Introduction of an efficient workflow for reliable Gibbs free energy differences and oxidation potentials in the catalytic cycle of ruthenium-based water oxidation catalyst (WOC) at low computational cost using GFN-xTB and DFT. *In silico* optimization of charge separating push-pull dyes for prevention of charge recombination. Simulations of electron and hole transfer in a dye-WOC photocatalytic complex. Quantum-classical semi-empirical description of a full photoanode system *in silico*.

Research Internship - *University of Massachusetts Amherst (UMass Amherst)*, USA 08/2016-12/2016
Supervisors Prof. Bret Jackson (Amherst), Prof. Geert-Jan Kroes (Leiden)
Simulation of Surface Lattice Vibrations on stepped surfaces with DFT based AIMD (using VASP program) and extracting site and temperature specific displacements for including phonon effects in reactive scattering simulations. Quantum dynamics of the scattering of methane from Ni(111) using the Reaction Path Hamiltonian.

Master Internship – *Universiteit Leiden (UL)*, The Netherlands 09/2015-07/2016
Supervisors Dr. Francesco Buda, Prof. Huub de Groot
Real-time simulations of photoinduced charge transfer in molecular complexes, using the non-adiabatic approaches of *Ehrenfest* dynamics and TDDFT-based Surface Hopping. Thorough investigation of coherent charge transfer in a pseudo base pair including determination of relevant molecular vibrations, isotope effect and dynamical symmetry breaking. Charge transfer in dimers and trimers of naphthalene diimide based dyes.

Research Assistant - ***Institute for Photonic Technology***, Jena 11/2014-12/2014
Supervisors Dr. Dana Cialla-May, Prof. Jürgen Popp
Further Lab-on-Chip SERS measurements on additional mycobacteria.

Bachelor Internship – ***FSU Jena***, ***Institute for Photonic Technology***, Jena 05/2014-09/2014
Supervisors Dr. Dana Cialla-May, Prof. Jürgen Popp
Detection and Classification of Mycobacteria using Lab-on-Chip Surface Enhanced Raman Spectroscopy (SERS). Synthesis of silver nanoparticles.

Student Research Assistant – ***Institute for Photonic Technology***, Jena 06/2013
Supervisors Prof. Jürgen Popp
Assisting in Raman measurements on the distribution of oleic acids in cell membranes and plasma.

Publications

§ Contributed Equally

*** Corresponding Author(s)**

C. Y. Chan, J. P. Menzel, Y. Dong, Z. Long, A. Waseem, X. Wu, Y. Xiao, J. Xie, E. Chow, S. Rakheja, V. S. Batista, Z. Mi, Y. Li*: "*Demystifying Metal-Assisted Chemical Etching of GaN and Related Heterojunctions*", *Appl. Phys. Rev.*, **2024**, 11(2), 021416

D. Nishiori, J. P. Menzel, N. Armada, E. A. Cruz, B. L. Nannenga, V. S. Batista, G. F. Moore*: "*Breaking a Molecular Scaling Relationship Using an Iron-Iron Fused Porphyrin Electrocatalyst for Oxygen Reduction*", *J. Am. Chem. Soc.,* **2024**, XXXX(XXX) XXX-XXX

J. A. Jayworth§, C. Decavoli§, M. D. Capobianco, J. P. Menzel, S. R. Adler, C. A. Kocoj, J. G. Freeze, R. H. Crabtree, P. Guo, V. S. Batista, G. W. Brudvig*: "*BODIPY Chemisorbed on SnO_2 and TiO_2 Surfaces for Photoelectrochemical Applications*", *ACS App. Mater. Interfaces*, **2024**, 16(12), 14841-14851

W. Lu§, H. Li§, J. P. Menzel, A. E. Cuomo, A. M. Nikolic, H. R. Kelly, Y. Shee, S. Sreekumar, F. Buono, J. J. Song, R. H. Crabtree, V. S. Batista, T. R. Newhouse: "*Enhanced Ligand Discovery through Generative AI and Latent-Space Exploration: Application to the Mizoroki-Heck Reaction*", *chemrxiv*, **2024**, 10.26434/chemrxiv-2024-hfw3p

W. J. Dong§, J. P. Menzel§, Z. Ye, I. A. Navid, P. Zhou, K. R. Yang, V. S. Batista*, Z. Mi*: *"Photoelectrochemical Urea Synthesis from Nitrate and Carbon Dioxide on GaN Nanowires"*, *ACS Catal.*, **2024**, 14(4), 2588-2596

A. E. Cuomo, S. Ibarraran, S. Sreekumar, H. Li, J. Eun, J. P. Menzel, P. Zhang, F. Buono, J. J. Song, R. H. Crabtree, V. S. Batista*, T. R. Newhouse*: "*Feed Forward Neural Network for Predicting Enantioselectivity of the Asymmetric Negishi Reaction*", *ACS Cent. Sci.*, **2023**, 9 (9), 1768-1774

M. L. A. Hakkenes, M. S. Meijer, J. P. Menzel, A. C. Goetz, R. Van Duijn, M. A. Siegler, F. Buda*, S. Bonnet*: "*Ligand Rigidity Steers the Selectivity and Efficiency of the Photosubstitution Reaction of Strained Ruthenium Polypyridyl Complexes*", *J. Am. Chem. Soc.*, **2023**, 145 (24), 13420-13434

J. P. Menzel*, Y. Boeije, T. M. A. Bakker, J. Belić, H. J. M. de Groot, L. Visscher, J. N. H. Reek, F. Buda*: *"In Silico Optimization of Charge Separating Dyes for Solar Energy Conversion"*, *Chem. Sus. Chem.,* **2022**, 15: e202200594

J. Belić, A. Förster, J. P. Menzel, F. Buda, L. Visscher*: "*Automated Assessment of Redox Potentials for Dyes in Dye-Sensitized Photoelectrochemical Cells*", *Phys. Chem. Chem. Phys.,* **2022**, 24: 197-210; **Correction:** *Phys. Chem. Chem. Phys.,* **2023**, 25: 19266-19268

J. P. Menzel*, M. Kloppenburg, J. Belić, H. J. M. de Groot, L. Visscher, F. Buda*: "*Efficient Workflow for the Investigation of the Catalytic Cycle of Water Oxidation Catalysts: Combining GFN-xTB and Density Functional Theory*", *J. Comp. Chem.,* **2021**, 42 (*26*): 1885-1894

J. P. Menzel*, A. Papadopoulos, J. Belić, H. J. M. de Groot, L. Visscher, F. Buda*: "*Photoinduced Electron Injection in a Fully Solvated Dye-Sensitized Photoanode: A Dynamical Semi-Empirical Study*", *J. Phys. Chem. C,* **2020**, 124 (*51*): 27965-27976

J. Belić*, B. van Beek, J. P. Menzel, F. Buda, L. Visscher*: *"Systematic Computational Design and Optimization of Light Absorbing Dyes", J. Phys. Chem. A*, **2020**, *124 (31)*:6380-6388

J. P. Menzel, H. J. M. de Groot, F. Buda*: "*Photoinduced Electron Transfer in Donor-Acceptor Complexes: Isotope Effect and Dynamic Symmetry Breaking*", *J. Phys. Chem. Lett*., **2019**, *10(21)*:6504-6511

H. Guo, J. P. Menzel, B. Jackson*: "*Quantum dynamics studies of the dissociative chemisorption of CH 4 on the steps and terraces of Ni(211)*", *J. Chem. Phys*., **2018**, *149(24)*:244704

H. Chadwick, H. Guo, A. Gutiérrez-Gonzaléz, J. P. Menzel, B. Jackson, R. D. Beck: "*Methane Dissociation on the Steps and Terraces of Pt(211) Resolved by Quantum State and Impact Site*", *J. Chem. Phys.*, **2018**, *148 (1)*: 014701

Awards and Scholarships

Sustainable Energy & Fuels Poster prize at the ***International Solar Fuels Conference*** July 29th 2021

Best Chemistry *Zij-instromer* student prize by the ***Leiden Institute of Chemistry (LIC)*** Sept. 06th 2016

LUF Internationaal StudieFonds (LISF) scholarship by the ***Leids Universiteits Fonds (LUF)*** June 28th 2016

Holland Scholarship by the ***Dutch ministry of Education, Culture and Science*** and ***UL*** April 15th 2016

LUSTRA+ scholarship by ***UL*** March 10th 2016

Temporary Fellow of the **Studienstiftung des deutschen Volkes** Jan. 2012-Oct. 2013

Conference Contributions and Presentations

Renewable Energy: Solar Fuels, Gordon Research Conference 2024 Ventura, California, USA
Poster presentation Feb. 04th-09th 2024

Renewable Energy: Solar Fuels, Gordon Research Seminar 2024 Ventura, California, USA
Poster presentation Feb. 03rd-04th 2024

ARO MURI Review Meeting 2022 — Ann Arbor, Michigan, USA
Poster presentation — Oct. 31st– Nov. 1st 2023

Energy Sciences Institute Retreat 2023 — New Haven, Connecticut, USA
Poster presentation — Sep. 21st 2023

49th IUPAC World Chemistry Congress/ CHAINS 2023 — Den Haag, The Netherlands
Contributed Talk — Aug. 20th-25th 2023

Invited Presentation — Zurich, Switzerland
at Luber group, University of Zurich — Aug. 15th 2023

ARO MURI Review Meeting 2022 — Online
Poster presentation — Nov. 1st-2nd 2022

Chemistry as Innovating Science (CHAINS) 2021 — Online
Poster presentation — Dec. 7th-8th 2021

Computational Methods in Photosynthesis — Online
Poster presentation — Sept. 30th - Oct. 1st 2021

International Solar Fuel Conference and Young Conference (ISF2021) — Online
Poster, **Poster prize** — July 26th-29th 2021

Dutch Photochemistry Days — Online
Contributed Talk — May 10th, May 17th 2021

Physics at Veldhoven 2021 — Online
Contributed Talk — January 18th-20th 2021

Chemistry as Innovating Science (CHAINS) 2020 — Online
Contributed Talk — December 08th-09th 2020

Chemistry as Innovating Science (CHAINS) 2019 — Veldhoven, The Netherlands
Poster presentation — December 10th-11th 2019

HRSMC Lustrum Symposium 2019 — Amsterdam, The Netherlands
Contributed Talk — November 14th-15th 2019

Solar to Products Symposium — Eindhoven, The Netherlands
Poster presentation — November 06th 2019

Reedijk Symposium 2019 — Leiden, The Netherlands
Poster presentation — October 25th 2019

10th Triennial Congress of the — Tromsø, Norway
International Society for Theoretical Chemical Physics (ISTCP 2019) — July 11th-17th 2019
Poster presentation

CTC Symposium 2019 — Amsterdam, The Netherlands
Poster presentation — March 26th 2019

Chemistry as Innovating Science (CHAINS) 2018 — Veldhoven, The Netherlands
Contributed Talk — December 03rd-05th 2018

HRSMC Symposium 2018 — Leiden, The Netherlands
Poster presentation — November 15th 2018

Photoinduced Processes in Embedded Systems (PPES) conference — Pisa, Italy
Poster presentation — June 24th-27th 2018

Student Supervision

4 Leren Onderzoeken (LO) students	2 weeks
3 HRSMC master student projects short rotation	1-2 months
5 master student thesis projects	6-10 months
1 Colloquium/Literature study student	3 months
Co-supervision of undergraduate student (thesis project)	6 months
Co-supervision of 3 PhD students	12-18 months/ongoing

Teaching Experience

Exercise preparation and teaching of **Theoretical Chemistry Exercise Lectures** for 3rd year Molecular Science and Technology students	11/02-17/03/2020
Preparation and teaching of **computational exercises** for the **Lorentz Center summer school in Multi-Scale Modelling**	17/06/2019
Exercise preparation and teaching of **Theoretical Chemistry Exercise Lectures** for 3rd year Molecular Science and Technology students	23/04-11/06/2019
Assistant for **Organic Chemistry Lab Course** at the LIC for 1st year Biopharmaceutical Science students (full time)	17/02-01/03/2019
Assistant for **Organic Chemistry Lab Course** at the LIC for 1st year Biopharmaceutical Science students (full time)	19/02-16/03/2018
Student Assistant at the *Faculty of Chemistry and Earth Sciences, FSU Jena* in **Inorganic Chemistry Lab Course** for 1st year Medical students (full time)	02-03/2014

Languages

GERMAN:	**Native**	ENGLISH:	**Fluent (CEFR C2)**
DUTCH:	**Good (CEFR B1)**	FRENCH:	**Good (CEFR B1)**
NORWEGIAN:	**Basic (CEFR A2)**	LATIN:	**Latinum**

Software and Computer Skills

Software for Chemical modelling:

Amsterdam Density Functional (ADF)
Amsterdam Modelling Suite (AMS)
OCTOPUS
Car-Parinello MD (CPMD)
Surface Hopping using Arbitrary Coupling (SHARC)
Vienna ab initio Simulation Package (VASP)
Gaussian
CP2K
Dftb+

Programming Languages and OS:

Linux/UNIX
BASH
Python
Fortran (Basics)