Tom Demeyere

tom.dmre@gmail.com tomdemeyere.github.io tom-demeyere-091144b9 tomdemeyere

Education

University of Southampton, PhD in Computational Chemistry — Feb 2025

- Coupling of Modern Computational Techniques to Study the Oxygen Reduction Reaction

University of Lille/Jagiellonian University, Master in Theoretical Chemistry — 2020

- First year: "Molecular Dynamics and Chemical Reactivity"
- Second year: "Advanced Spectroscopy in Chemistry" (ASC) done via Erasmus+

University of Lille, Bachelor in Physics and Chemistry — 2018

Research Experience

Doctoral Research *University of Southampton, School of Chemistry* — 2020 – 2024

- Developed a Grand-Canonical Monte Carlo code to predict catalyst oxidation
- Bridged the gap between thermodynamic and kinetic aspects of the Oxygen Reduction Reaction overpotential by making use of ML models with fundamental chemistry principles, establishing a new framework for catalyst behavior prediction
- Conceptualized novel research projects aiming to perform a thorough comparison between state-of-the-art solvation models by computing electrode capacitances, workfunctions, and solvation energies at metal-electrolyte interfaces.
- Partnered with Johnson Matthey, a global catalyst manufacturer, to bridge our computational predictions with experimental validation
- Created a framework using combinatorial optimization to identify stable crystal structures for solid electrolytes and applied locality-sensitive hashing algorithms to achieve $O(n)$ time classification of 200M+ structures

Graduate Research *Jagiellonian University, Faculty of Chemistry* — 2019 – 2020

- Developed framework to generate physically motivated initial configurations for solvent molecules in computational simulations
- Applied semi-empirical computational methods and successfully predicted water dissociation on TiO_2 Rutile low-index surfaces
- Computed binding energies and workfunction changes upon adsorption of croconic acid on semi-conductor surfaces for photocatalytic applications using the DFT+U implementation in the VASP software.

Honors Awards & Fellowships

Johnson Matthey Industrial PhD Fellowship, *University of Southampton* — 2020 – 2024

International Mobility Grant, *French Department of Education* — 2019 – 2020

Erasmus+ Scholarship for International ASC Master, *Lille University* — 2019

Erasmus Fellowship for Research Internship, *Jagiellonian University* — 2019

Merit Scholarship (Bourse de Mérite), *French Department of Education* — 2014 – 2017

Open-source Contributions

Quansino (Author) — github.com/quansino

- Modular Monte Carlo Python code for sampling atomic configurations built upon ASE a core library, the code allows users to quickly build specific atomistic simulations they need
- The code have been developed following best coding practices, with thorough unit-testing and comprehensive documentation.

Atomic Simulation Environment (Developer) gitlab.com/ase

- Frequently contributed to the development via various bugfixes and adding new functionalities such as new molecular dynamics thermostats and input/output interfaces for various DFT codes
- Familiar with the inner workings of ASE, a core computational chemistry library, enabling me to quickly integrate computational frameworks for specific academic projects

Quantum Accelerator (Contributor) github.com/quacc

- Implemented multiple recipes for DFT codes and increased compatibility with workflow engines e.g. Parsl
- Proficient with workflow engines enabling rapid deployment of large-scale concurrent workflows

Publications

Bridging Oxide Thermodynamics and Site-Blocking: A Computational Study of ORR Activity on Platinum Nanoparticles Dec 2024

Tom Demeyere, Tom Ellaby, Misbah Sarwar, David Thompsett, Chris-Kriton Skylaris

10.1021/acscatal.5c00321 (ACS Catalysis)

A Comparison of Modern Solvation Models for Oxygen Reduction at the Pt(111) Interface Nov 2024

Tom Demeyere, Chris-Kriton Skylaris

10.1021/acs.jpcc.4c04924 (The Journal of Physical Chemistry C)

Multi-scale Modeling and Experimental Investigation of Oxidation Behavior in Platinum Nanoparticles Oct 2024

Tom Demeyere, Husn-Ubayda Islam, Tom Ellaby, Misbah Sarwar, David Thompsett, Chris-Kriton Skylaris

10.26434/chemrxiv-2024-72hfg (In submission to RSC Physical Chemistry Chemical Physics)

A Workflow for Identifying Viable Crystal Structures with Partially Occupied Sites Applied to the Solid Electrolyte Cubic Li7La3Zr2O12 Nov 2023

Julian Holland, ***Tom Demeyere***, Arihant Bhandari, Felix Hanke, Victor Milman, Chris-Kriton Skylaris

10.1021/acs.jpclett.3c02064 (The Journal of Physical Chemistry Letters)

Conferences

Tom Demeyere, Tom Ellaby, Misbah Sarwar, David Thompsett, Chris-Kriton Skylaris (Apr 2024), Video recording: *Oxidation of Realistic Platinum Nanoparticles*, JMAC, Warwick, UK

Tom Demeyere, Tom Ellaby, Misbah Sarwar, David Thompsett, Chris-Kriton Skylaris (Mar 2024), Poster: *Unraveling the Oxidation of Realistic Platinum Nanoparticles using Linear Scaling DFT and Modern Forcefields*, CCP9, Chester, UK

Tom Demeyere, Tom Ellaby, Misbah Sarwar, David Thompsett, Chris-Kriton Skylaris (Apr 2023), Poster: *Degradation of platinum nanoparticles by oxidation using coupled computational methods*, JMAC, Warwick, UK

Tom Demeyere, Tom Ellaby, Misbah Sarwar, David Thompsett, Chris-Kriton Skylaris (Aug 2022), Poster: *Coupling of computational methods to study platinum based electrocatalysts under realistic conditions*, Psi-k Conference, Lausanne, Switzerland

Tom Demeyere, Tom Ellaby, Misbah Sarwar, David Thompsett, Chris-Kriton Skylaris (Mar 2022), Short oral presentation & Poster: *DFT simulations comparing Oxygen Reduction Reaction mechanism on Platinum 111 surface and nanoparticles*, JMAC, Warwick, UK

Tom Demeyere, Tom Ellaby, Misbah Sarwar, David Thompsett, Chris-Kriton Skylaris (Jan 2022), Poster: *DFT simulations comparing Oxygen Reduction Reaction mechanism on Platinum 111 surface and nanoparticles*, UKCC, Loughborough, UK

Teaching & Mentoring

ONETEP Masterclass July 2024

- Provided intensive one-on-one mentoring to graduate students, enabling them to successfully implement ONETEP DFT code in their research projects
- Designed and delivered a comprehensive course on scientific Python programming and the ASE-ONETEP inter-

face, including hands-on demonstrations and oral presentation

CHEM2034: Digital Chemistry *University of Southampton* Jan 2022 – June 2022

- Collaborated on developing an educational Jupyter Notebook implementing numerical solutions to the Schrödinger equation for the He atom
- Provided one-on-one mentoring during workshops, helping students understand and implement quantum mechanical calculations

CHEM2025: Introduction to Programming *University of Southampton* Sept 2021 – Dec 2021

- Mentored students during practical Python workshops, guiding and helping them throughout the process.

Technologies

Programming Languages: Python, Julia, Fortran, Bash

Libraries: ASE, pymatgen, NumPy, SciPy, PyTorch, pandas, Matplotlib, scikit-learn, pytest, quacc

Software: Quantum Espresso, VASP, ONETEP, LAMMPS, JDFTx

Techniques: Core AI/ML techniques, Sampling techniques (MD, MC), DFT, Kinetic Modeling, Electrochemistry, Github Actions, HPCs

Languages

French: Native

English: Fluent

Additional Achievements

- Delivered presentations across multiple research groups, promoting research reproducibility through Jupyter Notebooks and best practices in scientific computing
- Helped over 1M students with Mathematics and Physical Chemistry on Socratic, a science Q&A platform
- Achieved five-star ranking in HackerRank problem-solving track with 200+ solved challenges