

David Simonne

Postdoctoral Associate

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📍 Cambridge, MA, USA

PROFILE

PhD in physics, expertise in the study of bulk and surface crystalline structures with synchrotron imaging, diffraction, and spectroscopy techniques.


Developer of collaborative Python packages, and analysis pipelines used for data reduction, simulation, and analysis.

I currently aim at understanding the impact of radiation on the structural materials of nuclear reactors. I am also interested in the complex heterogeneous catalytic reactions in the ammonia and oxygen system, and in the optimisation of solid-state batteries.

WORK EXPERIENCE

Postdoctoral associate

02/2024 – present
Cambridge, USA

Massachusetts Institute of Technology, PI: Dr. Ericmoore Jossou 

Studying radiation damage in structural materials *operando* with a combined simulation + imaging approach. Project leader for synchrotron-based diffraction imaging techniques and electron microscopy imaging. Material science and chemistry lab EHS responsible, graduate student supervision, industry collaboration with GE Vernova

Scientific presentations: MRS Spring meeting - Honolulu (2026), MRS Fall meeting - Boston (2025), MRS Spring meeting - Seattle (2025), Coherence - Helsingborg (2024)

PhD student

11/2020 – 01/2024
Gif sur Yvette,
France

SOLEIL - CEA Grenoble, PI: Dr. A. Coati, Dr. A. Resta, Dr. M-I Richard

Thesis title: *Catalytic properties at the nanoscale probed by surface X-ray diffraction and coherent diffraction imaging.*

The ammonia oxidation reactions were studied *operando* on different platinum surfaces with a multi-technique approach, at ambient pressure. The importance of surface termination and surface oxides in the reaction selectivity was revealed.

A new Bragg Coherent Diffraction Imaging (BCDI) setup was implemented and optimized at the SixS beamline (SOLEIL) for combination with surface scattering techniques. Reproducible analysis workflows for Surface X-ray Diffraction (SXRD), X-ray Photoelectron Spectroscopy (XPS) and BCDI were developed.

Scientific presentations: MRS Spring meeting - Honolulu (2026), MRS Fall meeting - Boston (2025), Coherence - Helsingborg (2024), TMS Spring meeting - San Diego (2023), Coherence - Shanghai (2022), GDR CohereX - Marseille (2022), ESRF User Meeting - Grenoble (2022, 2023), SOLEIL User Meeting - Saclay (2022, 2023), Association Francaise de Crystallographie (2021)

Post-graduate research assistant (Assegno di ricerca)

01/2020 – 11/2020
Torino, Italy

University of Torino, PI: Dr. Elisa Borfecchia

Study of catalytic reactions at ambient pressure with spectroscopy techniques.

Development of the informatics tools supporting a new instrument for the study of catalysts with X-ray Absorption Spectroscopy (XAS).

Graduate research assistant (Master thesis)

04/2019 – 10/2019
Munich, Germany

Technical university of Munich, PI: Pr. Michael Leitner

Study of atomic ordering during phase transitions in high entropy Heusler alloys by neutron diffraction.

Development of refinement codes for neutron diffraction.

Graduate research assistant (Master 1)

Uppsala universitet, PI: Pr. Maximilian Wolff [✉](#)

Small Angle Neutron Scattering (SANS) study of micellar systems under stress.

05/2018 – 06/2018

Uppsala, Sweden

Undergraduate research assistant (COLABS)

Tohoku University, PI: Pr. Shinichiro Iwai

Studies at the Ultrafast Spectroscopy Laboratory about excitation intensity dependence of ultrafast carrier dynamics in GaAs and primary dynamics of photoinduced phase transition in V2O3.

2016 – 2017

Sendai, Japan

Undergraduate research assistant (Bachelor thesis)

FRM2, PI: Dr. Jean François Moulin [✉](#)

Design of a heating-cell and optimization of the experimental process for solid-liquid interfaces experiments inside the neutron reflectometer REFSANS.

05/2016 – 06/2016

Munich, Germany

Mailman

La Poste Française

Recurring summer jobs.

Avranches, France

Waiter

Restaurant Le Mouton Blanc

Recurring summer jobs.

Le Mont St Michel,

France

EDUCATION

PhD

Physique en Île de France (PIF), Université Paris-Saclay [✉](#)

X-ray / neutron interaction with matter, machine learning for 3D imaging, project management, synchrotron radiation.

2020 – 2024

Saclay, France

M.Sc Physics

Technical university of Munich [✉](#)

Curriculum focused on Material Science and Physics.

2017 – 2019

Munich, Germany

Cooperative Laboratory Study Program (COLABS)

Tohoku university [✉](#)

2016 – 2017

Sendai, Japan

Bachelor of Physics

Université de Rennes 1 [✉](#)

2014 – 2016

Rennes, France

SKILLS

Material characterisation

Expert in synchrotron diffraction / spectroscopy / imaging techniques (BP, BCDI, SXRD, DFXM, XAS, XCT). User of electron imaging techniques (SEM, FIB + STEM).

Scientific writing and presenting

LaTeX, Beamer.

International collaboration

Initiated and participates in long term collaborations within Europe and the USA.

Scientific communication

Held different projects to communicate about case studies to the non-expert public (Pint of Science, Open Science days).

Student supervision

Direct supervision of one graduate student at Paris-Saclay university, and three graduate students at MIT, resulting in second author publications.

Data analysis

2D and 3D data visualisation with Matplotlib, Bokeh, Jupyter Notebook, JupyterLab, Paraview. Reproducible workflows with standard data storage (hdf5, NeXuS), analysis pipelines in Python, BASH.

Daily usage of HPC and experience setting up analysis pipelines.

Simulation

X-ray scattering (PyNX), radiation damage (SRIM/TRIM)

Project management

Version control (git), focus on clear documentation, unit tests, and continuous integration.

Teaching

Practicals (88h) and tutorials (14h) to bachelor students at Université Paris-Saclay.

Practicals (4h) to bachelor students at MIT in 2025.

LANGUAGES

English

TOEFL, 109/120 (2018), main work language

German

B2

AWARDS

Best poster award

2025

MRS Fall meeting - Seattle

Multi-Scale Imaging of Corrosion and Hydrogen Embrittlement in Irradiated Nuclear Materials

Scholarship

2023

Marina Rocks

Funding for the JupyterCon conference.

Scholarship

2023

GDR CohereX

Funding for the TMS - San Diego conference.

Scholarship

2017

Fondation Université Rennes 1

Funding for an internship in Uppsala, Sweden.

Erasmus + scholarship

2016

University of Rennes 1

Fellowship, Tuition + monthly allowance for graduate studies at Tohoku University (Japan) in the graduate school of physics.

PUBLICATIONS

Transient Surface Oxides Form on Pt(111)—But Vanish During Ammonia Oxidation [↗](#)

2025

On arXiv - Under internal review

Simonne, D.; Coati A.; Vlad A.; Garreau Y.; M.I. Richard and Resta A.

Contribution: Original idea, Experimental design, Data collection, data reduction, data analysis, manuscript redaction.

Linking Surface Reconstructions to Catalytic Selectivity on Pt(100) during Ammonia Oxidation [↗](#)

2025

ACS Catalysis, 2026, 16

Simonne, D.; Coati A.; Vlad A.; Garreau Y.; M.I. Richard and Resta A.

Contribution: Original idea, Experimental design, Data collection, data reduction, data analysis, manuscript redaction. **IPF=13.1**

Dynamic Structural Changes of Ensemble and Single Supported Pt Particles During Ammonia Oxidation [↗](#)

2025

Applied Catalysis B: Environment and Energy, 2026, 383

Simonne, D.; M.I. Richard; Dupraz M.; Vlad A.; Garreau Y.; Chatelier C.; Voisin B.; Atlan C.; Yehya S.; Levi M.; Rabkin E.; Coati A. and Resta A.

Contribution: Experimental design, Data collection, data reduction, data analysis, manuscript redaction. **IPF=21.1**

X-ray irradiation induced strain relaxation of dewetted Ni particles on modified Si substrate [↗](#)

2025

Scripta Materiala 2026, 270

Simonne D.; Hultquist R.; Zhao J.; Resta A. and Jossou E.

Contribution: Original idea, Experimental design, Data collection, data reduction, data analysis, manuscript co-redaction. **IPF=5.6**

Multipurpose in situ cell design for 3D X-ray imaging of electrochemical processes [↗](#)

2025

Review of Scientific Instruments, 96

Hultquist R.; Simonne D.; Mondal S. and Jossou E.

Contribution: Cell design supervision and testing, manuscript co-redaction. **IPF=1.7**

- cdiutils: A python package for Bragg Coherent Diffraction Imaging processing, analysis and visualisation workflows** [↗](#) 2025
Zenodo
Atlan C.; [Simonne D.](#); Chatelier C.; Bellec E.; Olson K. and Deschamps M.
Contribution: Python code, SixS beamline integration, interactive visualisation tools.
- Capturing Catalyst Strain Dynamics during Operando CO Oxidation** [↗](#) 2024
ACS Nano 2024, 18
Grimes M.; Atlan C.; Chatelier C.; Bellec E.; Olson K.; [Simonne D.](#); Levi M.; Schüllli T. U.; Leake S. J.; Rabkin E.; Eymery J. and Richard M.I.
Contribution: Data collection, manuscript revisions. **IPF=16.1**
- gwaihir: Jupyter Notebook graphical user interface for Bragg Coherent Diffraction** [↗](#) 2022
Journal of Applied Crystallography - Computer Programs 2022, 55
[Simonne D.](#); Carnis J.; Atlan C.; Chatelier C.; Favre-Nicolin V.; Dupraz M.; Leake S. J.; Resta A.; Coati A. and M.I. Richard
Contribution: Original idea, Code development, manuscript redaction. **IPF=3**
- bcdi, tools for pre(post)-processing Bragg and forward coherent X-ray diffraction imaging data** [↗](#) 2022
Zenodo
Carnis J., Atlan, C., [Simonne, D.](#), Leake S., Dzhigaev D., Kishore K., Dupraz M., DeepSource Bot, Singaravelan K., and Richard M.I.
Contribution: Python code.
- Atomic Order along the Half-to Full-Heusler Transition in Ni_{1+x}MnSb** [↗](#) 2021
Physica Status Solidi B: Basic Solid State Physics 2021, 259
Neibecker P.; Xu X.; [Simonne D.](#); Hollender L.; Porcher F.; Senyshyn A.; Omori T.; Kainuma R.; Petry W. and Leitner M.
Contribution: Neutron diffraction data analysis, manuscript revisions. **IPF=1.8**
- Effect of manganese promotion on the activity and selectivity of cobalt catalysts for CO preferential oxidation** [↗](#) 2021
Applied Catalysis B: Environmental 2021, 297
Zhong L; Barreau M.; Chen D.; Caps V.; Haevecker M.; Teschner D.; [Simonne D.](#); Borfecchia E.; Baaziz W.; Šmíd B. and Zafeirato S.
Contribution: XANES data collection and analysis. Corresponding manuscript section redaction. **IPF=21.1**
- thorondor: a software for quick treatment and analysis for low energy XAS data** [↗](#) 2020
Journal of Synchrotron Radiation - Computer Programs 2020, 27
[Simonne D.](#); Martini A.; Signorile M.; Piovano A.; Braglia L.; Torelli P.; Borfecchia E. and Ricchiardi G.
Contribution: Original idea, Code development, manuscript redaction. **IPF=3**
- Time Resolved Polarised Grazing Incidence Neutron Scattering from Composite materials** [↗](#) 2019
Polymers 2019, 11
Wolff M.; Saini A.; [Simonne D.](#); Adlmann F. and Nelson, A
Contribution: Data analysis, manuscript revisions. **IPF=4.9**

ORGANISATIONS

MIT European Club

Board member - Student outreach and event chair

Organisation of the largest European career fair in north america, aiming at improving the recruitment of MIT graduates from European companies, and promoting European culture and values.

11/2024 – Present
Cambridge, USA