Msc. David Simonne PhD student



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D PUBLICATIONS

bcdi, tools for pre(post)-processing Bragg and forward coherent X-ray diffraction imaging data, *Zenodo* 🛛

2022

Carnis J., Atlan, C., Simonne, D.;, Leake S., Dzhigaev D., Kishore K., Dupraz M., DeepSource Bot, Singaravelan K., and Richard M.I. Contribution: code development.

Atomic Order along the Half-to Full-Heusler Transition in

Ni1+xMnSb, Physica Status Solidi B: Basic Solid State Physics ⊿ 2021

Neibecker, P.; Xu, X.; Simonne, D.; Hollender, L.; Porcher, F.; Senyshyn, A.; Omori, T.; Kainuma, R.; Petry, W.; and Leitner, M. Contribution: data reduction and analysis.

Effect of manganese promotion on the activity and selectivity of cobalt catalysts for CO preferential oxidation,

Applied Catalysis B: Environmental 🛛

2021

Zhong, L; Barreau, M.; Chen, D.; Caps, V.; Haevecker, M.; Teschner, D.; Simonne, D.; Borfecchia, E.; Baaziz, W.; Šmíd, B.; Zafeirato, S. Contribution: data reduction and analysis.

THORONDOR: a software for quick treatment and analysis for low energy XAS data,

Journal of Synchrotron Radiation - Computer Programs 2020

D. H. Simonne, A. Martini, M. Signorile, A. Piovano, L. Braglia, P. Torelli, E. Borfecchia and G. Ricchiardi. Contribution: code development and writing.

B PROFILE

PhD candidate in Physics, focused on the study of heterogeneous catalysts with synchrotron techniques. Specialized probing in material surfaces and bulk utilizing X-rays methods. Familiar with 3D image processing with Python. Author of Python packages and data analysis pipelines used for data reduction and analysis at Large Scale Facilities.

SKILLS

International • • • • • collaboration

Initiated and participates in several international projects.

Python • • • • • • Data reduction, analysis, program development.

GIT • • • • • Familiar with version control and team-collaboration.

Scientific • • writing LaTeX, Office suite

Scientific ● ● ● ● presentation

PROJECTS

EAGLES 2 Interactive data analysis softwares in Jupyter Notebook, international collaboration, optimized for computing clusters (JupyterHub) at Large Scale Facilities.

Time Resolved Polarised Grazing Incidence Neutron Scattering from Composite materials, *Polymers*

2019

Wolff, M.; Saini, A.; Simonne, D.; Adlmann, F.; Nelson, A. Contribution: data reduction and analysis.

PROFESSIONAL EXPERIENCE

PhD student,

SOLEIL - CEA Grenoble, Dr. A. Coati, Dr. A. Resta, Dr. M-I Richard 11/2020 – present | Gif sur Yvetter, France

- Image nanostructures to probe in situ and operando conditions.
- Understand the structural phenomena and link them to their **activity**, **selectivity**, **reusability** and **sustainability**.

Scientific project on Pt nanocatalysts used for the Ammonia oxidation, studied *via* Bragg Coherent Diffraction Imaging (BCDI) and Surface X-ray Diffraction (SXRD).

- Gwaihir ☑, program for the analysis of BCDI data.
- Co-tutor at the 2022 ESRF User Meeting (BCDI ID01).
- Oral presentation at the 2022 SOLEIL User Meeting.
- Poster presentation at the AFC conference 2021.

Research assistant, University of Torino, Dr. Elisa Borfecchia

01/2020 - 11/2020 | Torino, Italy

MOSCATo project: Cutting-edge X-ray methods and models for the understanding of surface site reactivity in heterogeneous catalysts and sensors.

- **Study of heterogeneous catalysis** with X-Ray Absorption Spectroscopy.
- *Thorondor* ≥, program for the analysis of soft X-Ray Absorption Spectroscopy data.

Intern, Technical university of Munich, Dr. Michael Leitner

04/2019 - 10/2019 | Munich, Germany

Master thesis: "Atomic ordering in Heusler alloys and neutron diffraction".

Analysis and refinement of models on neutron diffraction data sets by the means of process modelling and least squares regression. All programs were written in Python.

Intern, Uppsala universitet, Dr. Maximilian Wolff 🛛

05/2018 - 06/2018 | Uppsala, Sweden

- Analysis of Small-Angle Neutron Scattering (SANS) data on micellar systems.
- First approach to data analysis, large-scale facilities datasets and writing for publishing.

Personal website 🛛

Online detailed CV with extra documents.



English ● ● ● ● ● ■ TOEFL (109/120, 2018)

French Native	••••
German B2	••••
Italian ^{B1}	••••
Japanese	• • • • •

COURSES

HERCULES 🛛

2022

School on Neutrons, X-ray Synchrotron Radiation, and Free Electron Laser for condensed matter studies.

X-ray interaction with matter

Familiar with Neutron and Xray diffraction, X-ray absorption spectroscopy, Xray photoelectron spectroscopy, Crystallography.

Programming languages

Online classes on Python, Bash, Linux, MPI, HTML, CSS, website hosting (*openclassrooms.com*, MOOC).

Intern, Tohoku University, Pr. Dr. Shinichiro Iwaï

2016 – 2017 | Sendaï, Japan

Group research projects at the Ultrafast Spectroscopy Laboratory:

- Excitation Intensity Dependence of Ultrafast Carrier Dynamics in GaAs
- Primary Dynamics of Photo-Induced Phase Transition in V2O3

Intern, FRM2, Dr. Jean François Moulin 🗷

05/2016 - 06/2016 | Munich, Germany

- Design of a heating-cell used inside a diffractometer
- Optimization of the experimental process for solid-liquid interfaces experiments inside the neutron reflectometer REFSANS.

Mailman, La Poste Française

Avranches, France Summer job as mailman, three years in a row.

EDUCATION

PhD, *Physique en Île de France (PIF), Université Paris-Saclay* 2020 – present | Saclay, France

- Training at Collège de France, HERCULES school, ENS Paris-Saclay.
- Teaching physics labs at Université Paris-Saclay.

M.S. Physics, Technical university of Munich 🛛

2017 – 2019 | Munich, Germany

- Joint degree with Université de Rennes 1 (Fr) / University of Turin (It).
- Crystallography, solid-state physics and chemistry, quantum physics, metals and alloys, spectrocopy, and numerical methods.

COLABS, Tohoku university 🛛

2016 – 2017 | Sendaï, Japan

Physics, materials science, and engineering courses. Japanese culture and language.

Bachelor of Physics, Université de Rennes 1 🛛

2014 - 2016 | Rennes, France

Electromagnetism, classical and quantum mechanics, thermodynamics, solid-state physics, optics, crystallography, nuclear physics, mathematics for physics.

awards

Scholarship, Fondation

Université Rennes 1 2017

Awarded for an internship in Uppsala, Sweden.

Erasmus + scholarship,

University of Rennes 1 2016

Awarded by a selection committee for a specific collaboration between the University of Rennes 1 and Tohoku University.