David Simonne

Post-doctoral researcher

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AWARDS

Scholarship, *Marina Rocks*
2023
Funding for the JupyterCon conference.

Scholarship,
Fondation Université Rennes 1
2017
Funding for an internship in Uppsala, Sweden.

Erasmus + scholarship,
University of Rennes 1
2016
Funding for a one year exchange program at Tohoku University.

Scholarship, *GDR CohereX*
2023
Funding for the TMS - San Diego conference.

PROFILE

PhD in physics, focused on the study of heterogeneous catalysts with synchrotron techniques.
Specialized in multi-technique probing of surfaces and bulk utilizing diffraction and spectroscopy X-rays methods.

Author of Python packages and analysis pipelines used for data reduction and analysis.

Currently at MIT as post-doctoral associate, in the nuclear science and engineering group, aiming at studying defects in nuclear materials with synchrotron techniques.

PUBLICATIONS

Gwaihir: Jupyter Notebook graphical user interface for Bragg Coherent Diffraction,
Journal of Synchrotron Radiation - Computer Programs
2022
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: code development and writing.

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., Singaravelan K., and Richard M.I.
Contribution: project navigation, 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.

Time Resolved Polarised Grazing Incidence Neutron Scattering from Composite materials, *Polymers*
2019
Wolff, M.; Saini, A.; Simonne, D.; Adlmann, F.; Nelson, A.

SKILLS

International collaboration ●●●●○
Initiated and participates in long term collaborations within Europe and the USA.

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

Scientific writing and presenting ●●●●●
LaTeX, Beamer, Office suite.

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

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

Teaching ●●●●○
Taught practicals (88h) and tutorials (14h) to physics bachelor students at Université Paris-Saclay. Experience with bachelor/master student supervision.

COURSES

HERCULES, *ESRF, SOLEIL, PSI*
2022
School on neutrons and X-ray synchrotron radiation for condensed matter studies.

NanOperando, *Polytechnique*
2022
Summer school on techniques for studies at the nanoscale.

MOOC
2023
Increase performance with computing clusters / Scientific integrity in research / Understanding nanoscience.

Contribution: data reduction and analysis.

PROFESSIONAL EXPERIENCE

PhD student,
SOLEIL - CEA Grenoble, Dr. A. Coati, Dr. A. Resta, Dr. M-I Richard
11/2020 – 12/2023 | Gif sur Yvette, France
Thesis title: *Catalytic properties at the nanoscale probed by surface x-ray diffraction and coherent diffraction imaging.*

A new Bragg Coherent Diffraction Imaging (BCDI) setup was implemented at SixS (SOLEIL) and optimized. Reproducible workflows for Surface X-ray Diffraction (SXRD), X-ray Photoelectron Spectroscopy (XPS) and BCDI were developped. Ambient pressure catalytic reaction were studied on platinum surfaces with different surface X-ray diffraction techniques at three different synchrotrons.

Scientific presentations were held at TMS - San Diego - USA (2023), Coherence conference - Shanghai - China (2022), GDR CohereX - Marseille (2022), ESRF User Meeting - Grenoble (2022, 2023), SOLEIL User Meeting - Saclay (2022, 2023), AFC conference (2021).

Research assistant (Assegno di ricerca),
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.

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

Intern, *Technical university of Munich, Dr. Michael Leitner*
04/2019 – 10/2019 | Munich, Germany
Atomic ordering in Heusler alloys studied with neutron diffraction.

Intern, *Uppsala universitet, Dr. Maximilian Wolff*
05/2018 – 06/2018 | Uppsala, Sweden
Small Angle Neutron Scattering study of micellar systems under stress.

Intern, *Tohoku University, Pr. Dr. Shinichiro Iwaï*
2016 – 2017 | Sendaï, Japan
Studies at the Ultrafast Spectroscopy Laboratory about excitation intensity dependence of ultrafast carrier dynamics in GaAs and primary dynamics of photoinduced phase transition.

Intern, *FRM2, Dr. Jean François Moulin*
05/2016 – 06/2016 | Munich, Germany
Design of a heating-cell used inside a diffractometer and optimization of the experimental process for solid-liquid interfaces experiments inside the neutron reflectometer REFSANS.

Mailman, *La Poste Française*
Avranches, France

Waiter, *Restaurant Le Mouton Blanc*
Le Mont St Michel, France

PROJECTS

EAGLES
Interactive data analysis softwares compatible with Jupyter Notebook. Based on international collaboration, optimized for computing clusters (JupyterHub).

Personal website - detailed CV

LANGUAGES

English *(TOEFL, 109/120, 2018)*

French *(Native)* • **German** *(B2)*

Italian *(B1)* • **Japanese** *(N4)*

EDUCATION

PhD, *Physique en Île de France (PIF), Université Paris-Saclay*
2020 – present | Saclay, France
- Training at College de France, HERCULES school, ENS Paris-Saclay, Polytechnique

M.Sc Physics, *Technical university of Munich*
2017 – 2019 | Munich, Germany
Curriculum focused on Material Science and Physics.

Cooperative Laboratory Study Program (COLABS),
Tohoku university
2016 – 2017 | Sendaï, Japan

Bachelor of Physics, *Université de Rennes 1*
2014 – 2016 | Rennes, France