David Simonne

Post-doctoral 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.

Developper 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.

PROFESSIONAL EXPERIENCE

Postdoctoral associate 02/2024 – present
Massachusetts Institute of Technology, Dr. Ericmoore Jossou Cambridge, USA
Studying radiation damage in structural materials with a combined simulation + imaging approach. Project leader for synchrotron-based imaging techniques (CDI / tomography / DFXM) and electron imaging (SEM, FIB+STEM). Material science and chemistry lab EHS responsible, graduate student supervision.
Board member of the MIT european club.

Scientific presentations: Coherence - Helsingborg (2024).

PhD student 11/2020 – 12/2023
SOLEIL - CEA Grenoble, Dr. A. Coati, Dr. A. Resta, Dr. M-I Richard Gif sur Yvette, France
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). Reproducible analysis workflows for Surface X-ray Diffraction (SXRD), X-ray Photoelectron Spectroscopy (XPS) and BCDI were developped.

Scientific presentations: 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) 01/2020 – 11/2020
University of Torino, Dr. Elisa Borfecchia Torino, Italy
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).

Intern (Master thesis) 04/2019 – 10/2019
Technical university of Munich, Dr. Michael Leitner Munich, Germany
Study of atomic ordering during phase transitions in high entropy Heusler alloys by neutron diffraction.

Intern (Master 1) 05/2018 – 06/2018
Uppsala universitet, Dr. Maximilian Wolff Uppsala, Sweden
Small Angle Neutron Scattering study of micellar systems under stress.

Intern (COLABS) 2016 – 2017
Tohoku University, Pr. Dr. Shinichiro Iwaï 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 (Bachelor thesis) 05/2016 – 06/2016
FRM2, Dr. Jean François Moulin Munich, Germany
Design of a heating-cell and optimization of the experimental process for solid-liquid interfaces experiments inside the neutron reflectometer REFSANS.

EDUCATION

PhD 2020 – present
Physique en Île de France (PIF), Université Paris-Saclay Saclay, France
X-ray / neutron interaction with matter, machine learning for 3D imaging, project management, synchrotron radiation.

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

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

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

SKILLS

Material characterisation
Expert in synchrotron diffraction / spectroscopy / imaging techniques (CDI, 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
Supervision of Master and PhD student at MIT and Paris-Saclay university.

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.

Simulation
X-ray scattering (PyNX), molecular dynamics (LAMMPS/OVITO), 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.

LANGUAGES

English ●●●●●
TOEFL, 109/120, 2018

French ●●●●●
Native

German ●●●●○
B2

Italian ●●●○○
B1

Japanese ●●○○○
N4

AWARDS

Scholarship 2023
Marina Rocks
Funding for the JupyterCon conference.

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

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

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

PUBLICATIONS

Capturing Catalyst Strain Dynamics during Operando CO Oxidation 07/2024
ACS Nano
Grimes M., Atlan C., Chatelier C., Bellec E., Olson K., Simonne D., Levi M., Schülli T. U., Leake S. J., Rabkin E., Eymery J. and Richard M. I.
Contribution: data collection, scientific analysis

Gwaihir: Jupyter Notebook graphical user interface for Bragg Coherent Diffraction 2022
Journal of Synchrotron Radiation - Computer Programs
Simonne D., Carnis J., Atlan C., Chatelier C., Favre-Nicolin V., Dupraz M., Leake S. J., Resta A., Coati A. and Richard M.I.
Contribution: code development, writing.

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

Atomic Order along the Half-to Full-Heusler Transition in Ni1+xMnSb 2021
Physica Status Solidi B: Basic Solid State Physics
Neibecker P., Xu X., Simonne D., Hollender L., Porcher F., Senyshyn A., Omori T., Kainuma R., Petry W., and Leitner M.
Contribution: data reduction, scientific analysis.

Effect of manganese promotion on the activity and selectivity of cobalt catalysts for CO preferential oxidation 2021
Applied Catalysis B: Environmental
Zhong, L; Barreau, M.; Chen, D.; Caps, V.; Haevecker, M.; Teschner, D.; Simonne, D.; Borfecchia, E.; Baaziz, W.; Šmíd, B.; Zafeirato, S.
Contribution: XANES data reduction, scientific analysis.

THORONDOR: a software for quick treatment and analysis for low energy XAS data 2020
Journal of Synchrotron Radiation - Computer Programs
D. H. Simonne, A. Martini, M. Signorile, A. Piovano, L. Braglia, P. Torelli, E. Borfecchia and G. Ricchiardi.
Contribution: code development, writing.

Time Resolved Polarised Grazing Incidence Neutron Scattering from Composite materials 2019
Polymers
Wolff, M.; Saini, A.; Simonne, D.; Adlmann, F.; Nelson, A.
Contribution: data reduction, scientific analysis.