Arnaud Allera | Atomic-scale materials modelling

Molecular dynamics | Materials science | Machine-learning

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Employment

IRSN, PSN-RES/SEMIA/LSMA — **Cadarache, FR**
Permanent Researcher — *2024 –*
In charge of steels ageing studies. Materials science, simulation, machine-learning.

CEA, DES-SRMP — **Saclay, FR**
Postdoctoral researcher — *2022 – 2024*
New structural analysis methods based on descriptors. *PI: M.C. Marinica.*

Univ. Lyon, IRSN, INSA Lyon — **Lyon, FR**
PhD in Physics — *2018 – 2022*
Multi-scale modelling of screw dislocations glide and pinning in Fe-C steel.
Supervision: D. Rodney, M. Perez, F. Ribeiro .

Deakin University, IFM — **VIC, Australia**
Master thesis — *2018*

Skills

Computing: Python, C++ 11, F90, JS | HPC | Docker

AI/ML: Pytorch, Tensorflow, SkLearn, Force-Fields models (SNAP, MILADY)

Simulation: LAMMPS (MD, free energy calculations), KMC, VASP (DFT), ASE

Communications

Publications: *Neighbors Map: an Efficient Atomic Descriptor for Structural Analysis using Neural Networks.*, A. Allera, A. M. Goryaeva, P. Lafourcade, J-B Maillet, M.-C. Marinica, Computational Materials Science 231, 112535 (2024).

Robust crystal structure identification at extreme conditions using a density-independent spectral descriptor and supervised learning., P. Lafourcade, J.-B. Maillet, C. Denoual, E. Duval, A.Allera, A.M. Goryaeva, M.-C. Marinica Computational Materials Science 230, 112534 (2023).

Carbon-induced strengthening of bcc iron at the atomic scale, A. Allera, F. Ribeiro, M. Perez, D. Rodney, Physical Review Materials, 6(1) 013608 (2022).

Conference talks: MMM 10-11, COSIRES '22, MRS '20, GDR IAMAT, Plasticité ('21–'24)

Invited talks/seminars: GDR ModMat, 2024; LaSie, La Rochelle, 2023; ICAMS, Ruhr University Bochum, Germany, 2021

Education

Engineering Degree in Materials Science — **Lyon, FR**
INSA Lyon — *2013–2018*