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Centre Interdisciplinaire de Nanoscience de Marseille
Campus de Luminy, Aix-Marseille Université
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Education/Employment

- 10/18-CNRS Researcher, section 5 (tenured, international entrance competition with national jury)
- 04/17-06/18 Postdoc, Theoretical Division, Los Alamos National Laboratory *Supervisor: Dr D Perez*
- 03/15-02/17 EUROFusion Fellow, CCFE, UKAEA, Oxfordshire, UK *Supervisor: Prof SL Dudarev*

- 09/11-03/15 Imperial College PhD, Physics *Prof AP Sutton FRS. Materials Design & Blackett Prizes*
- 09/10-07/11 Imperial College MSc, Theory and Simulation of Materials, Distinction *Top Mark in Year*
- 10/06-07/10 Oxford University MPhys, Physics, 1st Class *First generation university student. Made Scholar then Exhibitioner for academic excellence. Departmental prize for excellence in laboratories*

Invited Visiting Fellowships

- Institute for Pure and Applied Mathematics, UCLA, USA, 2018, 2023, 2025 (*approx $15k/visit*)
- Institute for Mathematical and Statistical Innovation, University of Chicago, 2024 (*approx $10k/visit*)

Repeated invitations as visiting scholar at prestigious applied mathematics institutes in the USA Programs focused on materials informatics, machine learning and atomic simulation algorithms

Individual Awards

- Emerging Leader, Modelling in Materials Science and Engineering, IOP, 2021 and 2023
- Finalist, Rising Stars in Computational Materials Science, Elsevier, 2020
- Springer Outstanding PhD Award, Johnson-Matthey Thesis Prize and ICL Blackett Prize, 2015
- Materials Design Advanced Graduate Research Prize, Imperial College London, 2014

Selected Invited Presentations / Symposia in 2024

- Exploration in the structural and alchemical space of materials *MRS Fall, Boston, Dec.*
- Linear models in atomic ML: accuracy, uncertainty and beyond *General Physics Seminar, I'X, Nov.*
- AI in atomic simulation: what works and what might *Internat. Nuclear Consortium (MIT/Oxford), Nov.*
- *Ab-initio* accurate simulations of chemo-mechanics. *Engineering Seminar, U Oxford, Oct.*
- Coarse-graining of disordered systems at scale *Theoretical Chemistry Seminar, U Cambridge, Oct.*
- Deterministic model uncertainty *UQ day (three invited speakers) Max Planck Magdeburg, Aug.*
- *Ab-initio* accurate simulations of chemo-mechanics in tungsten *CIMTEC, Montecatini, Italy, June*
- Parallel, multi-scale simulation of irradiation annealing *(unavailable).* *COSIRIES 2024, Canada, June*
- Harnessing uncertainty in data-driven simulation *Mech. Eng. Seminar, U Michigan Ann Arbor, March*
- Descriptor dynamics as a novel simulation tool *Condensed Matter Th Seminar, Imperial College, Jan*
- Uncertainty from sampling incompleteness: known unknowns *UQ symposium, U Warwick, UK, Jan*

Community Service

- Associate Editor *(2023-) Computational Materials Science: machine learning, informatics specialist*
- Chair *COSIRES 2022 conference (120 worldwide participants)* sites.google.com/view/cosires2020
- Co-Chair *(w/ Manon Michel, CNRS) Probabilistic Sampling In Physics, Institut Pascal, Paris, 2023*
- Referee *PR[L/B/E/Materials], Acta/Scripta Materialia, Nat. Comms., NPJ, Adv. Mat., JCTC, JCIM …*

Funding Awarded as Sole/Lead Investigator *(PD=postdoc. Total 782k€ since 10/18)*

All amounts exclude permanent staff salaries. Typical success rate is 15% for ANR national grants.

- 04/24-04/28 ANR PRC "DaPredis" (PD & PhD, sub-PI: S Queyreau, LPSM, Paris) *Total: 270+180k€*
- 10/23-10/24 EMERGENCE@INP (PD on automatic differentiation in MD simulations) *Total: 90k€*
- 10/23-10/24 PTC, CEA (w/Dr L Ventelon, CEA Saclay PD using own QM/ML methods) *Total: 60k€*
- 03/20-08/22 ANR JCJC project "MeMoPAS" (sole PI, w/ 2-year PD) *Total: 202k€*
- 01/19-12/23 EUROFusion and GENCI/CINES CPU/GPU allocations *Total: approx. 120k€*

Selected Publications *(all corr. author) Google scholar 11/24: Citations = 1327, h-index = 21*

- Misspecification uncertainties in near-deterministic regression
  TDS and D Perez, arXiv:2402.01810,v5, to appear in Machine Learning: Science & Technology*
- Coarse graining and forecasting atomic material simulations with descriptors
  TDS, Physical Review Letters, 2023*
- Dislocation binding to defects in tungsten using hybrid ab initio-machine learning methods
  P Grigorev, AM Goryaeva, MC Marinica, JR Kermode, TDS*, Acta Materialia, 2023*
- Defining, calculating and converging observables of kinetic transition networks
  TDS and D.J. Wales, Journal of Chemical Theory and Computation 2020*
- Automated Calculation Of Defect Transport Tensors
  TDS and D. Perez, NPJ Computational Materials, 2020*
- Kink-limited Orowan strengthening explains the ductile to brittle transition of bcc metals
  TDS and S. L. Dudarev, Physical Review Materials (Editor's Suggestion), 2018*
- Self-optimised construction of transition rate matrices with Bayesian uncertainty quantification
  TDS and D. Perez, Physical Review Materials, 2018*
- Unsupervised calculation of free energy barriers in large crystalline systems
  TDS and M. C. Marinica*, Physical Review Letters, 2018*
- The classical mobility of highly mobile crystal defects
  TDS, S. L. Dudarev and A. P. Sutton, Physical Review Letters, 2014*

Open Source Software on `GitHub` *(sole/lead author unless stated, all MPI/C++/Python)*

- *`tomswinburne/POPS-Regression.git`* Fast parameter misspecification UQ for linear models
- *`marseille-matmol/LammpsImplicitDerivative.git`* Fast implicit differentiation for MD
- *`marseille-matmol/LML-retrain.git`* Hybrid DFT-MD/ML simulations (Acta Mat. 2023)
- *`tomswinburne/pafi.git`* Free energy evaluation for extended defects, `fix_pafi` in `LAMMPS`
- *`tomswinburne/tammber.git`* Massively parallel autonomous MD sampling (with D Perez, LANL)
- *`tomswinburne/PyGT.git`*: Graph Transformation (with D Kannan, MIT) pygt.readthedocs.io
- Multiple additions to `LAMMPS` molecular dynamics code (#17/223 contributors)

Postgraduate / Postdoctoral Student Supervision

- 12/20- Postdoc supervisor for Dr P Grigorev (2020-) and Dr Ivan Maliyov (2023-), CNRS/ CINaM
- 03/20- External PhD supervisor of R Dsouza, with Prof J Neugebauer, Max Planck Düsseldorf
- 06/19- Supervision of students (Y Sato and A Allera) using `PAFI` code, with Prof D Rodney, U Lyon
- 10/18- PhD co-supervisor of C Lapointe with Dr M-C Marinica, CEA Saclay
- 01/20-01/21 External MSc supervisor for D Kannan with Prof DJ Wales FRS, Univ. Cambridge

Teaching *Whilst CNRS positions are research-only, I strongly believe in the importance of teaching*

- 10/23 Designed and led program of hackathon projects for PhD students during role as co-chair of the "Probabilistic Sampling For Physics" Institut Pascal, see indico.ijclab.in2p3.fr/event/9042/
- 05/22 Course on atomistic simulations for CNRS MONACOSTE summer school. Designed cloud-based tutorial on regression methods for force field fitting : tinyurl.com/monacoste-cnrs-tutorial
- 11/20- Supervision of Physics MSc research projects for Aix-Marseille Université 'FunPhys` masters
- 04/17-07/17 Mentoring PhD students during summer program at Los Alamos National Laboratory
- 09/11-09/14 Undergraduate teaching and MSc/PhD supervision at Imperial College London
- 09/06-12/13 40+ students in private tuition and after school classes, both privately and for charity

References (*) / Collaborators

*Prof A P Sutton FRS, Imperial College London *(PhD Mentor, 4 articles)* a.sutton@imperial.ac.uk
*Prof D J Wales FRS, University of Cambridge *(2020-. PhD, MSc, 4 articles)* dw34@cam.ac.uk
*Prof Dr. J Neugebauer, Max Planck Eisenforschung *(2020-. PhD, 2 articles)* neugebauer@mpie.de
*Prof S L Dudarev, UKAEA Oxford *(postdoc mentor, 15-17, 6 articles)* sergei.dudarev@ukaea.ac.uk
Prof J R Kermode, U Warwick *(2020- 3 articles, code development)* j.r.kermode@warwick.ac.uk
Dr D Perez, Los Alamos National Lab. *(postdoc mentor 17-18, 5 articles)* danny_perez@lanl.gov
Dr M-C Marinica, CEA Saclay *(2018-. 2 PhDs, 7 articles)* mihai-cosmin.marinica@cea.fr