Thomas D Swinburne

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Research Interests

I design theoretical and computational methods to demonstrably extend the time and length scales accessible to atomic simulations of materials, with a primary interest in dislocation plasticity and rare event kinetics. All useful methods are approximate; my approach is to rigorously quantify uncertainty and use this to autonomously manage computational effort. This requires a parsimonious use of machine learning techniques for application to challenging, real-world problems. Results include:

- **QM/ML:** on-the-fly machine learning potentials to embed *ab initio* regions in large-scale atomic simulations, for e.g. complex segregation studies. Resolves long-standing issues (Acta Mat. 2023)
- **TAMMBER:** a rigorous bound on the influence of *unseen* atomic data on mesoscale models, used to autonomously control massively parallel, UQ-aware sampling e.g. defect diffusion (NPJ CM 2020)
- **PAFI :** a novel exact expression for vibrational free energy barriers, designed for application to extended defects which are untreatable with other methods. Implemented in LAMMPS (PRL 2018)

Employment

- **10/18-Present** CNRS Chargé de Recherche, Section 5 (tenured researcher, portable across France)
  03/23-06/23 : Senior Fellow, Institute for Pure and Applied Mathematics, UCLA, USA
- **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*

Education

- **09/11-03/15** Imperial College London, PhD *Physics, w/ Prof AP Sutton FRS. Blackett Prize 2015*
- **09/10-07/11** Imperial College London, MSc *Theory and Simulation of Materials. Top Mark in Year*
- **10/06-07/10** Oxford University, MPhys *Physics, 1st Class. Promotion to Scholar then Exhibitioner*

Funding Awarded *(Sole PI unless noted. PD=postdoc. Total 512k€ since CNRS hire in 10/18)*

- **10/23-10/24** EMERGENCE@INP (1-year PD for MD-UQ using automatic differentiation) *Total: 90k€*
- **10/23-10/24** PTC, CEA (w/ Dr L Ventelon. 1-year PD applying own QM/ML methods) *Total: 60k€*
- **03/20-08/22** ANR JCJC project "MeMoPAS" (w/ 2-year PD. 15% success rate) *Total: 202k€*
- **11/20-11/22** CNRS INP "Jeune Entrants" project joint with Dr B Sciacca *Total: 50k€*
- **01/19-12/23** EUROFusion and GENCI/CINES CPU/GPU allocations *Total: approx. 120k€*

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

Community Service

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

Selected Publications *(all corr. author) Google scholar, 03/23: Citations = 825, h-index = 17*

- 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
- Collective transport in the discrete Frenkel-Kontorova model
  TDS*, Physical Review E, 2013

Publicly Released Software *(sole / lead author unless stated, all parallel C++/Python)*
- `PAFI` : Free energy differences for extended defects. *github.com/tomswinburne/pafi*
- `TAMMBER` : Massively parallel autonomous MD sampling *github.com/tomswinburne/tammber*
- `QM/ML:` Hybrid DFT-MD/ML simulations *github.com/marseille-matmol/LML-retrain*
- `PyGT` : Python Graph Transformation *(MSc of D Kannan, U Cambridge)* pygt.readthedocs.io
- Multiple additions to `LAMMPS` code (#17 of 223 contributors) *github.com/lammps/lammps*

Selected Invited Presentations at International Conferences since 2021
- Data-driven coarse-graining and propagation of material simulations *IPAM, UCLA, 2023*
- Information transfer in multi-scale modelling *Mach Conference, Baltimore, 2023*
- Data-driven coarse-graining and propagation of material simulations *TMS Spring, San Diego, 2023*
- Exploration the structural and alchemical space of materials *World Congress on Comp. Mech. 2022*
- Exploration of material defects and nanoparticles *Multiscale Materials Modelling, Baltimore 2022*
- Defect thermodynamics at scale: high-throughput or high-accuracy *MRS Fall, Boston 2021*
- Sampling diffusion and plasticity in alloys *SIAM Materials Science, Bilbao, 2021*

Postgraduate / Postdoctoral Student Supervision
- 12/20- Postdoc supervisor for Dr P Grigorev, Centre Interdisciplinaire de Nanoscience de Marseille
- 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 and communication; I have actively sought to instruct students via MSc projects and summer schools*
- 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

Additional Interests / Skills
- Advanced listening, intermediate spoken and written French (working language)
- Founder and lead designer, Hawthorn Rucksacks, 2014-2018. (Closed during emigration from UK)
- Hobbies: guitar and mandolin (jazz and folk), sport climbing, cycling.

References / Collaborators
Prof A P Sutton FRS, Imperial College London *(PhD Supervisor)* a.sutton@imperial.ac.uk
Prof S L Dudarev, University of Oxford / UKAEA *(postdoc mentor 15-17)* sergei.dudarev@ukaea.ac.uk
Prof Dr. Joerg Neugebauer, Director, Max Planck Eisenforschung Düsseldorf *neugebauer@mpie.de*
  Collaborator since 01/20, one article in print to date. Co-supervision of PhD since 06/21
Prof D J Wales FRS, University of Cambridge *dw34@cam.ac.uk*
  Collaborator since 01/20. Co-supervision of PhD and MSc, four articles in print to date
Dr M-C Marinica, CEA Saclay *mihai-cosmin.marinica@cea.fr*
  Collaborator since 01/18. Co-supervision of two PhDs, seven articles in print to date
Dr D Perez, Los Alamos National Laboratory *(postdoc mentor 17-18)* *danny_perez@lanl.gov*
  Collaborator since 10/18, student co-supervision, three articles in print to date