Thomas D Swinburne

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Research Interests

Methods to extend time/length scales accessible to molecular dynamics simulations (MD) of materials. Primary interest in dislocation plasticity and metastable kinetics in crystalline solids. Results include:

- **PAFI (PRL 2018):** an exact expression for vibrational free energy barriers, designed for application to extended defects which are untreatable with other methods. Implemented in LAMMPS MD code.
- **TAMMBER (NPJ CM 2020):** massively parallel sampling of crystal defects, autonomously controlled by a novel, rigorous Bayesian bound on the influence of *unseen* atomic data on mesoscale models
- **QM/ML (Acta Materialia 2023):** custom machine learning force fields to embed *ab initio* simulations in large-scale MD studies of e.g. segregation phenomena. Resolves long-standing technical issues

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

- **04/24-04/28** ANR PRC "DaPredis" (PD & PhD, with 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" (w/ 2-year PD. 15% success rate) *Total: 202k€*
- **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, 07/23: Citations = 885, 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
- *Ab-initio* accurate simulations of chemo-mechanics in tungsten   *CIMTEC, Montecatini, 2024*
- 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, 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