Thomas D Swinburne

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Research Interests

Predicting plasticity and diffusive transport in metals through the development of advanced multiscale simulation methods, primarily at the atomic level. I extend theoretical models when possible and design principled data-driven methods where classical theories fail. In all cases I aim to establish robust mathematical foundations with clear uncertainty quantification. Recent results include

- Descriptor coarse-graining and forecasting (PRL 2023, sole author): I extended the scope of many body "descriptor" functions far beyond energy models to capture complex microstructures and enable error-controlled forecasts of simulation futures. *Funding as PI: ANR DAPREDIS*

- QM/ML (Acta Materialia 2023, last author): resolved long-standing problems to realise the grail of embedding small *ab initio* regions in general atomic simulations, for chemical accuracy only where needed. First applied to solute-dislocation binding. *Funding as PI: ANR MEMOPAS and CEA PTC.*

- TAMMBER (NPJ Comp Mat 2020, first author): unsupervised computational discovery of defect diffusion mechanisms with UQ, managed by rigorous bounds on influence of *unseen* atomic data. Established stability of A15 Laves clusters as embryonic fcc irradiation defects (Nat. Comms. 2023)

- PAFI (PRL 2018, first author): exact algorithm for vibrational free energy barriers, applicable to large systems (e.g. dislocations/twins), often untreatable with approximate methods. Implemented in the popular LAMMPS simulation package, with massively parallel job management in separate code.

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 Prize*
- 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*

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€*

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)*
- 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*
- Open source code multiple additions to LAMMPS molecular dynamics code (#17/223 contributors)
- Referee *PR[L/B/E/Materials], Acta/Scripta Materialia, Nat. Comms., NPJ, Adv. Mat., JCTC, JCIM …*

Selected Publications *(all corr. author) Google scholar 02/24: Citations = 1040, h-index = 19*

- 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*

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

Selected Invited Presentations at International Conferences since 2023

- Exploration in the structural and alchemical space of materials *MRS Fall, Boston, 2024*
- Data-driven coarse-graining and forecasting of atomic plasticity simulations *IMSI†, Chicago, 2024*
- Alchemical sampling through high-dimensional density estimation *CSMA, Giens, France, 2024*
- *Ab-initio* accurate simulations of chemo-mechanics in tungsten *CIMTEC, Montecatini, Italy, 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*

† : invited as long-term participant/visiting scholar at prestigious applied mathematics institutes

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*

- 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 *(PhD Supervisor, 4 articles)* a.sutton@imperial.ac.uk
Prof S L Dudarev, UKAEA Oxford *(postdoc mentor, 15-17, 6 articles)* sergei.dudarev@ukaea.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
Prof Dr. J Neugebauer, Max Planck Eisenforschung *(2020-. PhD, 2 articles)* neugebauer@mpie.de
Prof D J Wales FRS, University of Cambridge *(2020-. PhD, MSc, 4 articles)* dw34@cam.ac.uk
Prof J R Kermode, U Warwick *(2020- 3 articles, code development)* j.r.kermode@warwick.ac.uk