Thomas D Swinburne

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Centre Interdisciplinaire de Nanoscience de Marseille
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Employment

- 10/18-Present CNRS Chargé de Recherche, Section 05: Structure and Dynamics of Matter
  Tenured, portable research fellowship awarded via international `concours' (rank: 3/120, 5 recruited)
  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*
  09/17-12/17 : Junior Fellow, Institute for Pure and Applied Mathematics, UCLA, USA
- 03/15-02/17 EUROFusion Fellow, Culham Centre for Fusion Energy *Supervisor: Prof SL Dudarev*

Education

- 09/11-03/15 Imperial College London, PhD *Physics Dept. Supervisor: Prof AP Sutton FRS*
- 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 *(all individual/sole PI unless noted)*

- 10/23-10/24 "Emergence" PTC grant CEA (joint with Dr L Ventelon, 1-year postdoc) *Total: 60k€*
- 03/20-08/22 Agence Nationale de Recherche project MeMoPAS (with 2-year postdoc) *Total: 202k€*
- 04/21-04/22 IFERC - Broader Approach Supercomputer in Rokkasho 1.4MCPUh *Total: 20k€*
- 11/20-11/22 CNRS INP "Jeune Entrants" project joint with Dr B Sciacca *Total: 50k€*
- 06/20-10/23 GENCI/CINES computational allocations, total approx. 3MCPUh, *Total: 50k€*
- 01/19-12/23 EUROFusion Computational Research Projects (inc. approx. 2.0MCPUh), *Total: 40k€*

Individual Awards

- Emerging Leader, Modelling in Materials Science and Engineering, IOP, 2021
- Finalist, Rising Stars in Computational Materials Science, Elsevier, 2020
- Springer Outstanding PhD Thesis Award, Johnson-Matthey Thesis Prize, June 2015
- Blackett Laboratory Industry Thesis Prize, January 2015
- Materials Design Advanced Graduate Research Prize, January 2014
- Director's prize for best overall result in MSc, October 2011

Selected Publications *(all corr. author) Google scholar, 09/22: Citations = 731, h-index = 14*

- Synergistic coupling in ab initio-machine learning simulations of dislocations
  P Grigorev, AM Goryaeva, MC Marinica, JR Kermode, TDS*, under review, 2022*
- Anharmonicity and uncertainty in thermally activated dynamics
  TDS, Computational Materials Science (Invited review for 'Rising Stars' award) 2021*
- Automated calculation of defect transport tensors
  TDS and D. Perez, NPJ Computational Materials, 2020*
- Anharmonic free energy of lattice vibrations in fcc crystals from a mean-field bond
  TDS, J. Janssen, M. Todorova, J. Neugebauer et al. PRB Rapid Communications, 2020*
- Defining, calculating and converging observables of kinetic transition networks
  TDS and D.J. Wales, Journal of Chemical Theory and Computation 2020*
- Machine learning surrogate models for prediction of point defect vibrational entropy
  C. Lapointe, TDS, S. Mallat, M-C Marinica*, et al. Physical Review 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*
- Fast, vacancy free climb of dislocation loops in bcc metals
  TDS, K. Arakawa, S. L. Dudarev et al., Scientific Reports, 2016*
- 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*

Book Publications

- Stochastic Dynamics of Crystal Defects *TDS, Outstanding Thesis Series, Springer, 2015*

Publicly Released Software *(sole author unless stated)*

- `Fix-PAFI` module and contributions to C++/Python API for `LAMMPS` MD code
  (C++ / Python) `github.com/lammps/lammps`
- `PAFI` : Calculation of free energy differences for defects in crystalline materials from MD simulations
  (C++11 / Python) `github.com/tomswinburne/pafi`
- `TAMMBER` : Massively parallel, autonomously managed Markov coarse graining of MD simulations
  (C++11 / Python, with D Perez, Los Alamos Lab) `github.com/tomswinburne/tammber`
- `BLaSa` : Bond Lattice Sampling *(with J Janssen, MPIE)* `github.com/tomswinburne/blasa`
- `PyGT` : Python Graph Transformation *(MSc of D Kannan, U Cambridge)* `pygt.readthedocs.io`

Selected Invited Presentations at International Conferences since 2018

- 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*
- Autonomous construction of Markov Models with accelerated methods *ICIAM, Valencia, 2019*
- Statistical modelling of the brittle-to-ductile transition *Multiscale Material Modelling, Osaka, 2018*
- Autonomous and optimal exploration of defect energy landscapes *COSIRES, Shanghai 2018*

Selected Invited Seminars / Visits since 2018

- GDR ModMat Seminar May 2018 and April 2021, GDR HEA Seminar, November 2021
- Group of Prof. David Wales FRS, Cambridge University, January 2020 *Visit: one week*
- Center for Predictive Modelling Seminar, Warwick University, January 2020 *Visit: two days*
- Computational Materials Design Seminar, Max Planck Düsseldorf, May 2019 *Visit: one week*
- Theoretical Chemistry Seminar, Cambridge University, February 2019 *Visit: one week*
- Applied Mathematics Seminar, Imperial College London, January 2019 *Visit: two days*
- Nuclear Materials Science Seminar, University Of Oxford, September 2018 *Visit: two days*
- Centre for Nonlinear Studies meeting on Rate Theory, Santa Fe, June 2018 *Visit: three days*

Community Service

- Co-Chair *Probabilistic Sampling In Physics, Institut Pascal, Paris Saclay, 2023*
- Senior Fellow and Workshop Organiser *New Mathematics for the Exascale, IPAM, UCLA, 2023*
- Minisymposium Organiser *Decision-making in large-scale material simulations, WCCM Japan 2022*
- Conference Chair / Lead Organiser *COSIRES 2022* `sites.google.com/view/cosires2020`
- Referee *PR[L/B/E/Materials], Acta/Scripta Materialia, Nat. Comms., NPJ, Adv. Mat., JCTC, JCIM …*

Teaching and Supervision *CNRS positions are research-only; I only supervise at present*

- 12/20- Postdoc supervisor for Dr P Grigorev, Centre Interdisciplinaire de Nanoscience de Marseille
- 11/20- Supervision of Physics MSc research projects for Aix-Marseille Université ‘FunPhys` masters
- 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
- 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 Skills / Employment

- Advanced listening, intermediate spoken and written French (working language)
- Founder and lead designer, Hawthorn Rucksacks, 2014-2017. (Closed during emigration from UK)

References

Prof A P Sutton FRS, Imperial College London *a.sutton@imperial.ac.uk*
Prof D J Wales FRS, University of Cambridge *dw34@cam.ac.uk*
Prof S L Dudarev, Culham Centre for Fusion Energy *sergei.dudarev@ccfe.ac.uk*
Dr M-C Marinica, CEA Saclay *mihai-cosmin.marinica@cea.fr*
Dr D Perez, Los Alamos National Laboratory *danny perez@lanl.gov*