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 post awarded via international `concours' (5 hires from 120 shortlisted)
  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, Culham Centre for Fusion Energy *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 *(All sole PI unless noted. Total of 422k€ since CNRS appointment in 10/18)*

- 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" (w/ 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. 2MCPUh, *Total: 50k€*
- 01/19-12/23 EUROFusion Computational Research Projects (inc. approx. 2.0MCPUh), *Total: 60k€*

Individual Awards

- Emerging Leader, Modelling in Materials Science and Engineering, IOP, 2021
- 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, 01/23: Citations = 786, h-index = 16*

- Dislocation binding to defects in tungsten using hybrid ab initio-machine learning methods
  P Grigorev, AM Goryaeva, MC Marinica, JR Kermode, TDS*, Acta Materialia, 2022*
- 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*
- 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 / lead author unless stated, mostly C++/Python)*

- Multiple additions to `LAMMPS` code (#17 of 223 contributors) *github.com/lammps/lammps*
- `PAFI` : Free energy differences for extended defects : *github.com/tomswinburne/pafi*
- `TAMMBER` : Massively parallel, autonomously managed Markov coarse graining of MD simulations *(C++11, with D Perez, Los Alamos and EXAALT project)* *github.com/tomswinburne/tammber*
- `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 *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*
- 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*

Postgraduate / Postdoctoral 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

Prof D J Wales FRS, University of Cambridge *dw34@cam.ac.uk*
Prof A P Sutton FRS, Imperial College London *a.sutton@imperial.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*