Thomas D Swinburne

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Employment

- 10/18- Chargé de Recherche CNRS, Physics section 05 "Structure and dynamics of matter"
  Tenured researcher position, awarded through competitive "concours" entrance examination.
- 04/17-06/18 Postdoc, Theoretical Division T-1, Los Alamos National Lab. USA *Sup.: Dr D Perez*
- 03/15-02/17 EUROFusion Fellow, UKAEA, Oxford, UK *Concours European. Sup.: Prof SL Dudarev*

Invited visiting scholar positions

- Institute for Pure and Applied Mathematics, University of California Los Angeles, 2018, 2023, 2025
- Institute for Mathematical and Statistical Innovation, University of Chicago, 2024
  Invited "long term" participant at prestigious institutes in the USA. Typical residence of 1-3 months with invited talks. Programs covering machine learning and parallel computation in materials science

Education

- 09/11-03/15 Imperial College, Physics, PhD "Stochastic Dynamics of Crystal Defects"
  Under Prof. AP Sutton FRS. Lauréat of three thesis prizes (see below)
- 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 student. Promoted to "Scholar" then "Exhibitioner". Departmental prize for excellence in laboratories.*

Individual Awards / Prizes

- "Research Excellence" award from CNRS (individual salary bonus, 2024-2027)
- "Emerging Leader", Modelling in Materials Science and Engineering, IOP, 2021 and 2023
- Finaliste, Rising Stars in Computational Materials Science, Elsevier, 2020
- Springer Outstanding PhD Award (Thèse publiée, ISBN 9783319200194) July 2015
- Johnson-Matthey Thesis Prize, Faculty of Natural Sciences, Imperial College London, June 2015
- Blackett Laboratory Industry Thesis Prize, Department of Physics, Imperial College, Jan 2015
- Materials Design Advanced Graduate Research Prize, Imperial College London, October 2014

Grants obtained as PI *(PD=postdoc)*

- 04/24-04/28 ANR PRC "DaPredis" (PD & PhD, sub-PI: S Queyreau, LPSM, Paris) *Total: 270+180k€*
- 10/23-10/24 EMERGENCE@INP CNRS (PD on automatic differentiation techniques) *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€*

Grant participation

- 10/24-10/29 CONNECT-NM European partnership on nuclear materials. Task leader on assessing grants and materials databases for ML/Informatics usage *Total: 15pm*
- 10/23-10/27 ANR PRC "YOSEMITE" PI Dr H Amara (HEA Nanoparticles) *Total: 12pm*
- 10/23-10/27 ANR PRC "HEBERTUNE" (He-W for nuclear materials) *Total: 12pm, PhD supervision*

Community Service

- **Associate Editor** *(2023-) Computational Materials Science: machine learning, informatics specialist*
- **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 …*

Teaching *Whilst CNRS posts are research-only, I actively seek teaching/mentorship opportunities*

- 09/23 Design of group hackathon in program at Institut Pascal, Paris-Saclay (see "conferences")
- 09/21 Design of course introducing forcefields as part of "MONACOSTE" summer school, Fréjus
- 11/20-**present** Supervision of Physics MSc projects for Aix-Marseille Université 'FunPhys` masters

- 04/17-07/17 Mentoring PhD students during summer program at Los Alamos National Laboratory
- 09/11-03/15 Undergraduate teaching and MSc/PhD supervision at Imperial College London
- 09/06-12/15 100+ students in private tuition and school classes, both privately and for charity

Supervision of Masters / Doctoral / Postdoctoral students
- 03/24- Co-directeur of thesis for E Frikha, with Dr J Mougenot, LPSM Paris Nord
- 10/23- Postdoc supervisor for Dr I Maliyov, CInaM Marseille
- 12/20-02/24 Postdoc supervisor for Dr P Grigorev, CInaM Marseille
- 03/20- PhD co-supervisor of R Dsouza, with Prof J Neugebauer, Max Planck Düsseldorf
- 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

Selected presentations / symposia in 2024 (* = décliné/indisponible)
- Exploration in the structural and alchemical space of materials *MRS Fall, Boston, Dec.*
- Coarse-graining of disordered systems at scale *Theoretical Chemistry Seminar, U Cambridge, Oct.*
- Alchemical sampling through high-dimensional density estimation* *CSMA, Giens, France, Sep.*
- Uncertainty in deterministic models *UQ in Simulation (three speakers) Max Planck Magdeburg, Aug.*
- *Ab-initio* accurate simulations of chemo-mechanics in tungsten *CIMTEC, Montecatini, Italy, June*
- Massively parallel, multi-scale simulation of irradiation defects* *COSIRIES, Queen's U, Canada, June*
- Harnessing uncertainty in data-driven simulation *Mech. Eng. Seminar, U Michigan Ann Arbor, March*
- Descriptor dynamics as a novel simulation tool *Condensed Matter Seminar, Imperial College, Jan*

Selected publications as first/corresponding author
Google scholar 31/5/24: Citations = 1124, h-index = 20
- Parameter uncertainties of imperfect models in the low noise regime
TDS and D Perez, arXiv:2402.01810, under review at PNAS*
- 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*

Software as sole / lead author
- `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

References (*= for Baxandall Fellowship)
*Prof D J Wales FRS, University of Cambridge *(2020-. PhD, MSc, 4 articles)* dw34@cam.ac.uk
*Prof A P Sutton FRS, Imperial College London *(PhD Supervisor)* a.sutton@imperial.ac.uk

Prof Dr. J Neugebauer, Max Planck Dusseldorf *(2020-. PhD, 2 articles)* neugebauer@mpie.de
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