Thomas D Swinburne

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Employment
- 10/18- CNRS Chargé de Recherche, Section 05: Structure and Dynamics of Matter
  Portable, tenured, research-only position awarded via national 'concours' competition (rank: 2nd/120)
  Host institution: Centre Interdisciplinaire de Nanoscience de Marseille (CINaM)
- 04/17-09/18 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 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 as PI / individual)*
- 03/20-07/23 Agence Nationale de Recherche JCJC project MeMoPAS (w/ 2-year postdoc), €200k
- 06/20-06/22 DARI computational allocation, €20k (1.8MCPUh)
- 01/19-03/21 EUROFusion Computational Research Project, €18k
- 09/17-12/17 Postdoctoral scholarship, Institute for Pure and Applied Mathematics, UCLA ($12k)

Individual Awards
- Finalist, Rising Stars in Computational Materials Science, Elsevier, 2020
- Postdoc presentation award, MRS Fall 2015
- 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 Journal Publications *(all sole/joint corresponding author)*

Google scholar, 03/21: Citations = 460, h-index = 12

- 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-optimized 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
- Computing energy barriers from QM/MM simulations through the virtual work principle
  TDS and J.R. Kermode, Physical Review B, 2017
- 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++ API for `LAMMPS` molecular dynamics (MD) code
  (C++ / Python) https://github.com/lammps/lammps, 2020
- `PAFI` : Calculation of free energy differences for defects in crystalline materials from MD simulations
  (C++11 / Python) https://github.com/tomswinburne/pafi, 2020
- `TAMMBER` : Massively parallel, autonomously managed Markov coarse graining of MD simulations
  (C++11 / Python. With D Perez, LANL) https://github.com/tomswinburne/tammber, 2020
- `BLaSa` : Bond Lattice Sampling and Analysis
  (C++ / Python. With J Janssen, MPIE) https://github.com/tomswinburne/blasa, 2020
- `PyGT` : Graph transformation in Python
  (Beta version with D Kannan, U Cambridge) https://pygt.readthedocs.io, 2020

Invited Presentations at International Conferences (2018-)
- Quantifying exploration in the energy landscapes of material defects
  Multiscale Materials Modelling: MMM2020, Baltimore 2021
- Diffusion and plasticity in alloys - convergence in configurational and chemical space
  SIAM Materials Science, Bilbao, 2021
- Automated calculation of defect transport tensors
  World Congress on Comp. Mechanics, January 2021 & US Congress on Comp. Mech., July 2021
- Autonomous construction of Markov Models from accelerated sampling methods
  Energy Landscapes, Belgrade, August 2019 & ICIAM, Valencia, 2019
- Using free energy calculations and statistical mechanics to probe the brittle-to-ductile transition
  Multiscale Materials Modelling: MMM2018, Osaka 2018
- Autonomous and optimal exploration of defect energy landscapes
  Computer Simulations of Irradiation Effects in Solids: COSIRES, Shanghai 2018

Invited Seminars / Visits (2018-)
- Center for Predictive Modelling Seminar, Warwick University, January 2020   *Duration: two days*
- Computational Materials Design Seminar, MPIE Dusseldorf, May 2019   *Duration: one week*
- Wales Group, Cambridge University, Febuary 2019 (Seminar) & January 2020   *Duration: two weeks*
- Applied Mathematics Seminar, Imperial College London, January 2019   *Duration: two days*
- GDR ModMat, Uncertainty Quantification for Materials Science, Paris, May 2018 *Duration: two days*

Community Service
- **Core Workshop Organiser**, New Mathematics for the Exascale, IPAM, UCLA, Spring 2023
- **Conference Chair**, COSIRES 2022 http://sites.google.com/view/cosires2020
- Referee for PR[L/B/E/Materials], Acta/Scripta Materialia, NPJ, Nat. Comms., Advanced Materials…

Teaching and Supervision
  CNRS positions are research-only; present teaching activity is through student supervision
- **12/20-07/22** Postdoc supervisor for Dr Petr Grigorev, CINaM
- **03/18-09/21** External PhD supervisor for Clovis Lapointe with Dr M-C Marinica, CEA Saclay
- **03/20-09/23** External PhD supervisor for Raynol Dsouza with Prof J Neugebauer, MPIE Dusseldorf
- **01/20-03/20** M2 project supervisor, Physics department, Aix-Marseille Université
- **01/20-01/21** External MSc supervisor for Deepti Kannan with Prof DJ Wales FRS, Univ. Cambridge
- **04/17-07/17** Mentoring PhD students during 12 week 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 at CINaM)
- Founder and lead designer, Hawthorn Rucksacks, 2014-2017. (Closed when emigrating from UK)

References
Prof S L Dudarev, Culham Centre for Fusion Energy   *sergei.dudarev@ccfe.ac.uk*
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*
Dr M-C Marinica, CEA Saclay   *mihai-cosmin.marinica@cea.fr*
Dr D Perez, Los Alamos National Laboratory   *danny.perez@lanl.gov*