Thomas D Swinburne

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CINaM, Campus de Luminy,
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Employment

- 10/2018- Tenured CNRS CRCN (Section 5), Centre Interdisciplinaire de Nanoscience de Marseille
- 04/2017 - 09/2018, Postdoc, T-1, Los Alamos National Laboratory (Supervisor: D Perez)
- 03/2015 - 02/2017, EUROFusion Fellow, Culham Centre for Fusion Energy (Supervisor: S Dudarev)

Education

- PhD, 09/2011 - 03/2015, Imperial College London (Physics/TSM CDT Advisor: Prof AP Sutton FRS)
- MSc, 09/2010 - 07/2011, Imperial College London (TSM CDT. Distinction, top mark in year)
- MPhys, 10/2006 - 07/2010, University of Oxford (4-Year Physics degree. 1st Class)

Funding Awarded (as PI / individual)

- 2020-2023: ANR JCJC project MeMoPAS (2-year postdoc), €200k
- 2020-2022: DARI computational allocation, €20k (1.8MCPUh)
- 2019-2020: EUROFusion WPMAT/IREMEV project, €18k
- 2016-2017: IPAM Postdoctoral Residency $12k

Individual Awards

- Finalist, Rising Stars in Computational Materials Science, Elsevier, 2020.
- Postdoc presentation award, MRS Fall 2015.
- Eurofusion research fellowship award (in addition to CCFE fellowship), December 2015.
- Springer Outstanding PhD Thesis Award, June 2015.
- 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 (as corresponding/sole author)

- 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 otherwise stated)

- `PAFI` : Projected Average Force Integrator (C++11 / Python)

https://github.com/tomswinburne/pafi.git, 2020

- `Fix-PAFI` module in `LAMMPS` package (allowing constrained dynamics for PAFI code, C++)

https://github.com/lammps/lammps.git, 2020

- `TAMMBER` : Temperature Accelerated Markov Models with Bayesian Estimation of Rates (C++11)

(with D Perez, LANL) https://github.com/tomswinburne/tammber.git, 2020

- `BLaSa` : Bond Lattice Sampling and Analysis (C++ / Python)

(With J Janssen, MPIE) https://github.com/tomswinburne/blasa.git, 2020

- `PyGT` : Graph transformation in Python

(With D Kannan, U Cambridge) https://pygt.readthedocs.io, 2020

Selected Invited Presentations

- Quantifying exploration in nanoparticle energy landscapes *MMM 2020 (postponed to 2021)*
- Automated calculation of defect transport tensors *WCCM 2020 (postponed to 2021)*
- Diffusion in chemically complex alloys *SIAM MS 2020 (postponed to 2021)*
- Uncertainty-driven massively parallel sampling of crystal defects *Energy Landscapes 2019*
- Autonomous construction of Markov Models from accelerated sampling methods *ICIAM 2019*
- Using free energy calculations and statistical mechanics to probe the bcc-BDT *MMM 2018*
- Autonomous and optimal exploration of defect energy landscapes *COSIRES 2018*
- Temperature accelerated rate matrix construction in the Parsplice framework *IPAM, UCLA, 2017*
- Fast, vacancy free climb of dislocation loops *Dislocations 2016*
- Using projection operators to understand dislocations *Advances in Nanoscale Phenomena, 2016*
- Simulations of dislocation motion at experimentally realistic stresses *TMS 2014*

Community Service

- Lead organiser, COSIRES 2020 (postponed to 2021) http://sites.google.com/view/cosires2020
- Conference chair at MRS Fall 2017/19, Boston, USA and Dislocations 2019, Haifa, Israel
- Referee for PR[L/B/E/Materials], Acta/Scripta Materialia, NPJ, Nat. Comms., Advanced Materials…
- Organisation committee (finance / accounts), Hermes 2012 Conference, London.

Teaching and Supervision

- 2020- Postdoc supervisor for P Grigorev and MSc supervisor for V Dabhi 2020-21, CINaM
- 2019- External PhD supervisor for C Lapointe with M-C Marinica, CEA Saclay, France
- 2020- External PhD advisor for R. Dsouza with Prof J Neugebauer, MPIE Dusseldorf, Germany
- 2020- External MSc supervisor for D Kannan with Prof DJ Wales FRS, University of Cambridge, UK
- 2017: Mentoring of PhD students during 12 week program at Los Alamos National Laboratory, USA
- 2011-14: Undergraduate teaching and MSc/PhD supervision at Imperial College London, UK
- 2006-13: 40+ students in private tuition and after school classes, both privately and for charity.

Additional Skills / Employment

- Intermediate spoken and written French.
- Research for Isis Innovations, Oxford (2007-2009). Design of electromagnetic fuel probes
- Founder and lead designer of rucksack company (Hawthorn Rucksacks).

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*