

Thomas D Swinburne

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CINaM, Campus de Luminy,
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Employment

- 10/18 - Tenured CNRS CRCN (Section 5), Centre Interdisciplinaire de Nanoscience de Marseille
- 4/17 - 9/18, Postdoc, T-1, Los Alamos National Laboratory (Supervisor: Dr D Perez)
- 3/15 - 2/17, EUROfusion Fellow, Culham Centre for Fusion Energy (Supervisor: Prof SL Dudarev)

Education

- PhD, 9/11 - 3/15, Imperial College London (Physics Dept. Supervisor: Prof AP Sutton FRS)
- MSc, 9/10 - 7/11, Imperial College London (Theory and Simulation of Materials. Top Mark in Year)
- MPhys, 10/06 - 7/10, Oxford University (4-Year Physics degree, 1st Class. First generation student)

Funding Awarded (*all as PI / individual*)

- 2020-2023: Agence Nationale de Recherche JCJC project MeMoPAS (w/ 2-year postdoc), €200k
- 2020-2022: DARI computational allocation, €20k (1.8MCPUh)
- 2019-2020: EUROfusion Research Project, €18k
- 2016-2017: Institute of Pure and Applied Mathematics (UCLA) 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.
- Promotion to Scholar then Exhibitioner whilst undergraduate, for excellence in examinations

Selected Journal Publications (*all as corresponding/sole author*)

From Google scholar, 25/02/21: Citations = 447, h-index = 12

- 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 (*total of 16 at international conferences since 2016*)

- Quantifying exploration in the energy landscapes of material defects
Multiscale Materials Modelling: MMM2020, Baltimore 2020→21
- Automated calculation of defect transport tensors
World Congress on Computational Mechanics, Paris 2020→21
- Diffusion and plasticity in complex alloys - convergence in configurational and chemical space
SIAM Materials Science, Bilbao, 2020→21
- Autonomous construction of Markov Models from accelerated sampling methods
International Conference on Industrial and Applied Mathematics: 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
- Fast, vacancy free climb of dislocation loops

Dislocations 2016, Ann Arbor, 2016

Community Service

- Core organiser, IPAM long program on exascale computation, spring 2023
- Conference Chair, COSIRES 2020→22 <http://sites.google.com/view/cosires2020>
- Referee for PR[L/B/E/Materials], Acta/Scripta Materialia, NPJ, Nat. Comms., Advanced Materials...

Teaching and Supervision

- 2020-22 Postdoc supervisor for P Grigorev 2020-22, CINaM
- 2018-21 External PhD supervisor for C Lapointe with M-C Marinica, CEA Saclay
- 2020-23 External PhD advisor for R. Dsouza with Prof J Neugebauer, MPIE Dusseldorf
- 2020-21 External MSc supervisor for D Kannan with Prof DJ Wales FRS, University of Cambridge
- 2017: Mentoring of PhD students during 12 week program at Los Alamos National Laboratory
- 2011-14: Undergraduate teaching and MSc/PhD supervision at Imperial College London
- 2006-13: 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 leaving UK)

References

Prof S L Dudarev, Culham Centre for Fusion Energy
Prof A P Sutton FRS, Imperial College London
Prof D J Wales FRS, University of Cambridge
Dr M-C Marinica, CEA Saclay
Dr D Perez, Los Alamos National Laboratory

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