

Thomas D Swinburne

swinburne@cinam.mrs-univ.fr
<http://tomswinburne.github.io>

CINaM, Campus de Luminy,
13288 Marseille,
FRANCE

Employment

- 10/18- Tenured CNRS CRCN (Section 5), Centre Interdisciplinaire de Nanoscience de Marseille
- 04/17 - 09/18, Postdoc, T-1, Los Alamos National Laboratory (Supervisor: Dr D Perez)
- 03/15 - 02/17, EUROfusion Fellow, Culham Centre for Fusion Energy (Supervisor: Prof SL Dudarev)

Education

- PhD, 09/11 - 03/15, Imperial College London (Physics Department. Advisor: Prof AP Sutton FRS)
- MSc, 09/10 - 07/11, Imperial College London (Theory and Simulation of Materials. Top Mark in Year)
- MPhys, 10/2006 - 07/2010, University of Oxford (4-Year Physics degree. 1st Class)

Funding Awarded (all as PI / individual)

- 2020-2023: ANR JCJC project MeMoPAS (2-year postdoc), €200k
- 2020-2022: DARL 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 (all 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 Parsplce 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

- 2020-22 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

- 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
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

sergei.dudarev@ccfe.ac.uk
a.sutton@imperial.ac.uk
dw34@cam.ac.uk
mihai-cosmin.marinica@cea.fr
danny.perez@lanl.gov