

Thomas D Swinburne

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

CINaM, Campus de Luminy,
13288 Marseille,
FRANCE

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.git>, 2020
- **PAFI** : Calculation of free energy differences for defects in crystalline materials from MD simulations
(C++) <https://github.com/tomswinburne/pafi.git>, 2020
- **TAMMBER** : Massively parallel, autonomously managed Markov coarse graining of MD simulations
(C++ / Python. 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
(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, February 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
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