Thomas D Swinburne

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

CINaM, Campus de Luminy, AMU
13288 Marseille,
FRANCE

Employment

- **10/18-Present** CNRS Chargé de Recherche, Section 05: Structure and Dynamics of Matter
  Portable, tenured research position awarded via 'concours' process (rank: 2nd/120, top 5 recruited)
  Institute: Centre Interdisciplinaire de Nanoscience de Marseille, Aix-Marseille Université
- **04/17-06/18** Postdoc, Theoretical Division, Los Alamos National Laboratory *Supervisor: Dr D Perez*
  09/17-12/17 : Resident scholar, Institute for Pure and Applied Mathematics, UCLA
- **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)* `github.com/lammps/lammps`
- `PAFI` : Calculation of free energy differences for defects in crystalline materials from MD simulations *(C++11 / Python)* `github.com/tomswinburne/pafi`
- `TAMMBER` : Massively parallel, autonomously managed Markov coarse graining of MD simulations *(C++11 / Python, with D Perez, Los Alamos Lab)* `github.com/tomswinburne/tammber`
- `BLaSa` : Bond Lattice Sampling *(with J Janssen, MPIE)* `github.com/tomswinburne/blasa`
- `PyGT` : Python Graph Transformation *(MSc of D Kannan, U Cambridge)* `pygt.readthedocs.io`

Invited Presentations at International Conferences since 2018

- Quantifying exploration of material defects and nanoparticles *MMM2020, Baltimore 2022*
- Sampling diffusion and plasticity in alloys *SIAM Materials Science, Bilbao, 2021*
- Automated calculation of defect transport tensors *World Congress on Comp. Mech. 2021*, *US Congress on Comp. Mech. 2021*
- Autonomous construction of Markov Models with accelerated methods *ICIAM, Valencia, 2019*, *Energy Landscapes, Belgrade, 2019*
- Statistical modelling of the brittle-to-ductile transition *Multiscale Materials Modelling, Osaka 2018*
- Autonomous and optimal exploration of defect energy landscapes *COSIRES, Shanghai 2018*

Selected Invited Seminars / Visits since 2018

- GDR ModMat, UQ for Materials Science, Paris, May 2018 and Seminar Series, April 2021 (online)
- Group of Prof. David Wales FRS, Cambridge University, January 2020 *Visit: one week*
- Center for Predictive Modelling Seminar, Warwick University, January 2020 *Visit: two days*
- Computational Materials Design Seminar, Max Planck Düsseldorf, May 2019 *Visit: one week*
- Theoretical Chemistry Seminar, Cambridge University, February 2019 *Visit: one week*
- Applied Mathematics Seminar, Imperial College London, January 2019 *Visit: two days*
- Nuclear Materials Science Seminar, University Of Oxford, September 2018 *Visit: two days*
- Centre for Nonlinear Studies meeting on Rate Theory, Sante Fe, June 2018 *Visit: three days*

Community Service

- Core Workshop Organiser *New Mathematics for the Exascale, IPAM, UCLA, Spring 2023*
- Conference Chair / Lead Organiser *COSIRES 2022* `sites.google.com/view/cosires2020`
- Referee *PR[L/B/E/Materials], Acta/Scripta Materialia, Nat. Comms., NPJ, Adv. Mat., JCTC, JCIM …*

Teaching and Supervision

CNRS positions are research-only; present teaching activity is through student supervision

- 12/20- Postdoc supervisor for Dr P Grigorev, Centre Interdisciplinaire de Nanoscience de Marseille
- 11/20- Supervision of Physics M2 (masters) research projects at Aix Marseille Université
- 03/20- External PhD supervisor of R Dsouza, with Prof J Neugebauer, Max Planck Düsseldorf
- 06/19- Supervision of students (Y Sato and A Allera) using `PAFI` code, with Prof D Rodney, U Lyon
- 10/18- PhD co-supervisor of C Lapointe with Dr M-C Marinica, CEA Saclay
- 01/20-01/21 External MSc supervisor for D 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)
- 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*