

# Thomas D Swinburne

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## Employment

- **10/18-Present** CNRS Chargé de Recherche, Section 05: Structure and Dynamics of Matter  
*Tenured, portable research fellowship awarded via international 'concours' (rank: 2<sup>nd</sup>/120, 5 recruited)*
- **04/17-06/18** Postdoc, Theoretical Division, Los Alamos National Laboratory *Supervisor: Dr D Perez*  
*09/17-12/17 : Resident, Institute for Pure and Applied Mathematics, Univ. California Los Angeles*
- **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, 1<sup>st</sup> Class. Promotion to Scholar then Exhibitioner*

## Funding Awarded (all individual/sole PI unless noted)

- **03/20-07/23** Agence Nationale de Recherche project MeMoPAS (with 2-year postdoc) *Total: €202k*
- **04/21-04/22** IFERC - Broader Approach Supercomputer in Rokkasho 1.4MCPUh *Total: €20k*
- **11/20-11/22** CNRS INP "Jeune Entrants" project joint with Dr B Sciacca *Total: €50k*
- **06/20-06/22** DARI computational allocation, 1.8MCPUh, *Total: €20k*
- **01/19-03/21** EUROfusion Computational Research Project 1.5MCPUh, *Total: €18k*

## Individual Awards

- Emerging Leader, Modelling in Materials Science and Engineering, IOP, 2021
- 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 Publications (all corr. author) Google scholar, 10/21: Citations = 547, h-index = 13

- 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-optimised 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++/Python API for LAMMPS MD code  
(C++ / Python) [github.com/lammps/lammps](https://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](https://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](https://github.com/tomswinburne/tamMBER)
- **BLaSa** : Bond Lattice Sampling (with J Janssen, MPIE) [github.com/tomswinburne/blasa](https://github.com/tomswinburne/blasa)
- **PyGT** : Python Graph Transformation (MSc of D Kannan, U Cambridge) [pygt.readthedocs.io](https://pygt.readthedocs.io)

## Invited Presentations at International Conferences since 2018

- Exploration the structural and alchemical space of materials *World Congress on Comp. Mech. 2022*
- Quantifying exploration of material defects and nanoparticles *MMM2020, Baltimore 2022*
- Descriptor Markov models for the prediction of plastic evolution *NAWA Workshop, Warsaw 2022*
- Defect thermodynamics at scale: high-throughput or high-accuracy *MRS Fall, Boston 2021*
- Sampling diffusion and plasticity in alloys *SIAM Materials Science, Bilbao, 2021*
- Automated calculation of defect transport tensors *US & World 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 Seminar May 2018 and April 2021, GDR HEA Seminar, November 2021
- 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, Santa Fe, June 2018 *Visit: three days*

## Community Service

- **Minisymposium Organiser** *Decision-making in large-scale material simulations, WCCM Japan 2022*
- **Core Workshop Organiser** *New Mathematics for the Exascale, IPAM, UCLA, Spring 2023*
- **Conference Chair / Lead Organiser** *COSIRES 2022 [sites.google.com/view/cosires2020](https://sites.google.com/view/cosires2020)*
- **Referee** *PR[L/B/E/Materials], Acta/Scripta Materialia, Nat. Comms., NPJ, Adv. Mat., JCTC, JCIIM ...*

## Teaching and Supervision *CNRS positions are research-only; I only supervise at present*

- 12/20- Postdoc supervisor for Dr P Grigorev, Centre Interdisciplinaire de Nanoscience de Marseille
- 11/20- Supervision of Physics MSc research projects for Aix-Marseille Université 'FunPhys' masters
- 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 summer 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 before emigration from UK)

## References

Prof A P Sutton FRS, Imperial College London

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Prof D J Wales FRS, University of Cambridge

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Prof S L Dudarev, Culham Centre for Fusion Energy

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