

Thomas D Swinburne

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Centre Interdisciplinaire de Nanoscience de Marseille
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Employment

- **10/18-Present** CNRS Chargé de Recherche, Section 05: Structure and Dynamics of Matter
Tenured, portable research post awarded via international 'concours' (5 hires from 120 shortlisted)
03/23-06/23 : Senior Fellow, Institute for Pure and Applied Mathematics, UCLA, USA
- **04/17-06/18** 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, w/ Prof AP Sutton FRS. Blackett Prize 2015*
- **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 sole PI unless noted. Total of 422k€ since CNRS appointment in 10/18)

- **10/23-10/24** "Emergence" PTC grant CEA (joint with Dr L Ventelon, 1-year postdoc) *Total: 60k€*
- **03/20-08/22** Agence Nationale de Recherche project "MeMoPAS" (w/ 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€*
- **06/20-10/23** GENCI/CINES computational allocations, total approx. 2MCPUh, *Total: 50k€*
- **01/19-12/23** EUROfusion Computational Research Projects (inc. approx. 2.0MCPUh), *Total: 60k€*

Individual Awards

- Emerging Leader, Modelling in Materials Science and Engineering, IOP, 2021
- Finalist, Rising Stars in Computational Materials Science, Elsevier, 2020
- Springer Outstanding PhD Award, Johnson-Matthey Thesis Prize and ICL Blackett Prize, 2015
- Materials Design Advanced Graduate Research Prize, Imperial College London, 2014

Community Service

- **Associate Editor** (2023-) *Computational Materials Science (Elsevier)*
- **Co-Chair** (w/ Manon Michel, CNRS) *Probabilistic Sampling In Physics, Institut Pascal, Paris, 2023*
- **Conference Chair** COSIRES 2022 (120 participants) *sites.google.com/view/cosires2020*
- **Referee** *PR[L/B/E/Materials], Acta/Scripta Materialia, Nat. Comms., NPJ, Adv. Mat., JCTC, JCM ...*

Selected Publications (all corr. author) Google scholar, 12/22: Citations = 771, h-index = 15

- Synergistic coupling in ab initio-machine learning simulations of dislocations
P Grigorev, AM Goryaeva, MC Marinica, JR Kermode, TDS*, under review, 2022*
- 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*
- 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 / lead author unless stated, mostly C++/Python*)

- Multiple additions to LAMMPS code (#17 of 223 contributors) github.com/lammps/lammps
- PAFI : Free energy differences for extended defects : github.com/tomswinburne/pafi
- TAMMBER : Massively parallel, autonomously managed Markov coarse graining of MD simulations (C++11, with D Perez, Los Alamos and EXAALT project) github.com/tomswinburne/tamMBER
- PyGT : Python Graph Transformation (*MSc of D Kannan, U Cambridge*) pygt.readthedocs.io

Selected Invited Presentations at International Conferences since 2018

- Data-driven coarse-graining and propagation of material simulations *IPAM, UCLA, 2023*
- Information transfer in multi-scale modelling *Mach Conference, Baltimore, 2023*
- Data-driven coarse-graining and propagation of material simulations *TMS Spring, San Diego, 2023*
- Exploration the structural and alchemical space of materials *World Congress on Comp. Mech. 2022*
- Exploration of material defects and nanoparticles *Multiscale Materials Modelling, Baltimore 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*
- Autonomous construction of Markov Models with accelerated methods *ICIAM, Valencia, 2019*
- Statistical modelling of the brittle-to-ductile transition *Multiscale Material 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*

Postgraduate / Postdoctoral Supervision

- 12/20- Postdoc supervisor for Dr P Grigorev, Centre Interdisciplinaire de Nanoscience de Marseille
- 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

Teaching *Whilst CNRS positions are research-only, I strongly believe in the importance of teaching and communication; I have actively sought to instruct students via MSc projects and summer schools*

- 11/20- Supervision of Physics MSc research projects for Aix-Marseille Université 'FunPhys' masters
- 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 Interests / Skills

- Advanced listening, intermediate spoken and written French (working language)
- Founder and lead designer, Hawthorn Rucksacks, 2014-2018. (Closed during emigration from UK)
- Hobbies: guitar and mandolin (jazz and folk), sport climbing, cycling.

References

Prof D J Wales FRS, University of Cambridge

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Prof A P Sutton FRS, Imperial College London

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Prof S L Dudarev, Culham Centre for Fusion Energy

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Dr M-C Marinica, CEA Saclay

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Dr D Perez, Los Alamos National Laboratory

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