Thomas D Swinburne

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Employment

- 08/25- Assistant Professor, Dept. Mechanical Engineering, University of Michigan, Ann Arbor
- 10/18-08/25 Chargé de Recherche, CNRS Physique, *visiting researcher (détachement) from 8/25*
- 04/17-06/18 Postdoc, Theoretical Division T-1, Los Alamos National Lab. USA *Sup.: Dr D Perez*
- 03/15-02/17 EUROFusion Fellow, UKAEA, Oxford, UK *European "Concours" Sup.: Prof SL Dudarev*

Invited visiting positions *(fully funded, residence of 1-3 months with invited talks)*

- Institute for Pure and Applied Mathematics, University of California Los Angeles, 2018, 2023, 2025
- Institute for Mathematical and Statistical Innovation, University of Chicago, 2024

Education

- 09/11-03/15 Imperial College, Physics, PhD "Stochastic Dynamics of Crystal Defects"
  Supervisor: Prof. AP Sutton FRS. Laureate of three thesis prizes (see below)
- 09/10-07/11 Imperial College MSc, Theory and Simulation of Materials, Distinction
  Top mark in year.
- 10/06-07/10 Oxford University MPhys, Physics, 1st Class *First generation student. Promoted to "Scholar" then "Exhibitioner". Departmental prize for excellence in laboratories.*

Individual Awards

- Research excellence award from CNRS Physique (physics division) covering 2024-2027
- Emerging Leader, Modelling in Materials Science and Engineering, IOP, 2021 and 2023
- Finalist, Rising Stars in Computational Materials Science, Elsevier, 2020
- Springer Outstanding PhD Award (Thesis published, ISBN 9783319200194), 2015
- Johnson-Matthey Thesis Prize, Faculty of Natural Sciences, Imperial College London, 2015
- Blackett Laboratory Industry Thesis Prize, Department of Physics, Imperial College, 2015
- Materials Design Advanced Graduate Research Prize, Imperial College London, 2014

Grants obtained as PI *(PD=postdoc. Excluding staff salaries. External investigator from 8/25)*

- 04/24-04/28 ANR Collaborative Grant (main PI, postdoc & PhD, 15% success rate) *Total: 450k€*
- 10/23-10/24 CNRS Physique grant for postdoc on automatic differentiation techniques *Total: 90k€*
- 10/23-10/24 CEA-CNRS grant for postdoc applying own QM/ML methods *Total: 150k€*
- 03/20-08/22 ANR Young Researcher Grant (sole PI, 2-year postdoc, 15% success) *Total: 202k€*
- 03/20-present Multiple national/international computational allocations *Total: approx 150k€ in-kind*

Grant participation *(pm=person months, travel+ancillary budget excluded)*

- 06/25-12/27 CNRS-IRSN MITI, ML models for irradiation damage, PIs: A Allera, D Rodney, TDS
- 10/24-02/28 ESPRC project on inverse design, PI: Prof J Kermode, U Warwick, UK. *Total: 4pm*
- 10/23-10/27 ANR PRC "YOSEMITE" PI Dr H Amara (HEA Nanoparticles) *Total: 12pm, PD co-sup.*
- 10/23-10/27 ANR PRC "HEBERTUNE" (He-W for nuclear materials) *Total: 12pm, PhD supervision*

Postgraduate supervision

- 2025- PhD co-supervision with Profs T Lelièvre and A Parmentier, Ecole des Ponts Paris Tech.
- 2025- Sole postdoc supervisor and PhD co-supervisor within ANR DAPREDIS project
- 10/24-02/28 PhD co-supervisor of G Simmons, with Prof J Kermode, U Warwick, UK
- 03/24-09/27 PhD co-supervisor of E Frikha, with Dr J Mougenot, LPSM Paris Nord
- 10/23-11/24 Sole postdoc supervisor for Dr I Maliyov, CINaM Marseille
- 12/20-02/24 Sole postdoc supervisor for Dr P Grigorev, CINaM Marseille
- 03/20-01/25 PhD co-supervisor of R Dsouza, with Prof J Neugebauer, Max Planck Düsseldorf
- 10/18-02/22 PhD co-supervisor of C Lapointe, with Dr M-C Marinica, CEA Saclay
- 01/20-01/21 External MSc supervisor of D Kannan, with Prof DJ Wales FRS, Univ. Cambridge

Invited seminars/colloquia/visits (as of March 2025, from CNRS appointment in 2018)

- Linearity in atomic machine learning *Condensed Matter Seminar, Ecole Polytechnique, 03/25*
- Forecasting MD with descriptors *Keynote, EU COST Action "Mecanano", 02/25*
- Data-driven coarse-graining of dislocations. *PMMH Seminar, ESPCI, Paris, 01/25*
- The many uncertainties in atomic machine learning *Evening Symposium, IPAM Arrowhead, 12/24*
- Linearity in atomic machine learning *Seminar Générale de Physique, Ecole Polytechnique, 11/24*
- AI in atomic simulation: what works & what might *MIT International Nuclear Eng. Colloquium 11/24*
- Ab-initio accuracy for plasticity and thermodynamics *Engineering Seminar, U Oxford, 10/24*
- Beyond the loss: misspecification uncertainties *Theoretical Chem. Seminar, U Cambridge, 10/24*
- Quantifying misspecification uncertainties *Hattrick-Simpers Seminar, U Toronto, (Zoom) 07/24*
- Quantifying misspecification uncertainties *Lawrence Livermore UQ Seminar, (Zoom) 06/24*
- Harnessing uncertainty in data-driven simulation *Mech. Eng. Seminar, U Michigan, 03/24*
- Descriptor dynamics as a new simulation tool *Condensed Matter Sem., Imperial College, 01/24*
- Autonomous convergence of defect diffusivities *GDR (France-wide network) HEA Seminar 11/21*
- Free energy computations in materials science *GDR (France-wide network) ModMat Seminar 04/21*
- Energy barriers in QM/ML *Center for Predictive Modelling Seminar, Warwick University, 01/20*
- Visit to group of Prof. David Wales FRS *Chemistry Department, Cambridge University, 01/20*
- Uncertainty in kinetic Monte Carlo *Materials Design Seminar, Max Planck Düsseldorf, 05/19*
- Massively parallel, uncertainty-aware sampling *Theoretical Chem. Seminar, U Cambridge, 02/19*
- Multiscale analysis of a dislocation model *Applied Mathematics, Imperial College London, 01/19*
- The brittle-to-ductile transition in bcc metals *Nuclear Materials Science Seminar, Univ. Oxford, 09/18*
- Massively parallel, uncertainty-aware sampling for materials *GDR ModMat Seminar 03/18*

Invited conference talks (as of March 2025, from CNRS appointment * = *not available*)

- *Title tba* *Comp. Materials Science, International Centre for Math. Sciences, U. Edinburgh, 11/25*
- *Title tba* *IPAM, UCLA, 9/25*
- *Title tba* *Fulfilling the Multiscale Promise in Materials, CECAM Conference, Lausanne, 3/25*
- Quantifying misspecification uncertainties* *APS March Meeting, Anaheim, 3/25*
- Quantifying misspecification UQ *UQ in multiphysics learning, appliedmldays.org, EPFL, 2/25*
- Exploration in the structural and alchemical space of materials *MRS Fall, Boston, 12/24*
- Uncertainty in deterministic models *UQ in Atomic Simulation, Max Planck Magdeburg, 8/24*
- *Ab-initio* accurate simulations of chemo-mechanics in tungsten *CIMTEC, Montecatini, Italy, 6/24*
- Massively parallel, multi-scale simulation of irradiation defects* *COSIRIES, Canada, 6/24*
- Quantifying misspecification uncertainties* *HetSys Conference, University of Warwick, 6/24*
- Alchemical sampling through high-dimensional density estimation* *CSMA, Giens, France, 5/24*
- Descriptor dynamics as a new simulation tool *Materials Informatics, IMSI, U Chicago, USA, 5/24*
- Ab-initio accuracy for plasticity and thermodynamics *Warwick-Jiao Tong UQ Conf., UK, 1/24*
- Data-driven coarse-graining and propagation of material simulations *IPAM, UCLA, 3/23*
- Information transfer in multi-scale modelling *Mach Conference, Baltimore, 4/23*
- Data-driven coarse-graining and propagation of material simulations *TMS Spring, USA 3/23*
- Exploration the structural and alchemical space of materials *W. Congress on Comp. Mech. 2/22*
- Quantifying exploration of material defects and nanoparticles *MMM2020, Baltimore, USA 10/22*
- Descriptor Markov models for the prediction of plastic evolution *NAWA Workshop, Warsaw 9/22*
- Defect thermodynamics at scale: high-throughput or high-accuracy *MRS Fall, Boston 11/21*
- Sampling diffusion and plasticity in alloys *SIAM Materials Science, Bilbao, 7/21*
- Automated calculation of defect transport tensors *US & World Congress on Comp. Mech. 6/21*
- Uncertainty-driven massively parallel sampling *Energy Landscapes, Belgrade, 8/19*
- Statistical mechanics of the brittle to ductile transition in bcc metals *Dislocations, Haifa, 7/19*
- Autonomous construction of Markov Models from accelerated sampling *ICIAM Valencia, 7/19*
- Statistical mechanics of the brittle to ductile transition of bcc metals *MMM 2018, Osaka, 10/18*
- UQ for rare event dynamics *Advances in Computational Statistical Physics, CIRM, France, 9/18*

Community Service / Leadership Roles

- European Project Lead for ML *(2024-2029) CONNECT-NM partnership, nuclear materials research*
- Associate Editor *(2023-) Computational Materials Science: machine learning, informatics specialist*
- Chair *COSIRES 2022 conference (120 worldwide participants)* sites.google.com/view/cosires2020
- Co-Chair *(w/ Manon Michel, CNRS) Probabilistic Sampling In Physics, Institut Pascal, Paris, 2023*
- Co-Chair *(w/ Jonathan Amodeo, CNRS) Plasticité, Marseille (c.f. 100 participants), Marseille, 2024*
- Symposium co-chair *organisation of thematic sessions at international meetings (MMM20, IPAM)*
- Referee *PR[L/B/E/Materials], Acta/Scripta Materialia, Nat. Comms., NPJ, Adv. Mat., JCTC, JCIM*

Teaching

- 08/25- ME382 Mechanical Behavior of Materials, Mech.l Engineering, U Michigan (class of ~100)
- 09/23 Design of group hackathon in program at Institut Pascal, Paris-Saclay (see "conferences")
- 09/21 Design of course introducing forcefields as part of "MONACOSTE" summer school, Fréjus
- 11/20-present Supervision of Physics MSc projects for Aix-Marseille Université 'FunPhys` masters
- 04/17-07/17 Mentoring PhD students during summer program at Los Alamos National Laboratory
- 09/11-03/15 Undergraduate teaching and MSc/PhD supervision at Imperial College London
- 09/06-12/15 100+ students in private tuition and school classes, both privately and for charity

Selected publications as corresponding author

Google Scholar, 08/25: h-index=23, citations=1831

- Score matching the descriptor density of states for model-agnostic free energy estimation
  TDS, C Lapointe, MC Marinica, to appear in Nature Communications, 2025*
- Parameter uncertainties of imperfect models in the low noise regime
  TDS and D Perez, Machine Learning: Science & Technology, 2025*
- Coarse graining and forecasting atomic material simulations with descriptors
  TDS, Physical Review Letters, 2023*
- Dislocation binding to defects in tungsten using hybrid ab initio-machine learning methods
  P Grigorev, AM Goryaeva, MC Marinica, JR Kermode, TDS*, Acta Materialia, 2023*
- Defining, calculating and converging observables of kinetic transition networks
  TDS and D.J. Wales, Journal of Chemical Theory and Computation 2020*
- Automated Calculation Of Defect Transport Tensors
  TDS and D. Perez, NPJ Computational 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*
- 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*

Software as sole / lead author `github.com/tomswinburne`

Typically Python/JaX/C++/MPI. Own codes deployed on petascale HPC machines in US and EU

- `PAFI` : Free energy differences for extended defects. `github.com/tomswinburne/pafi`
- `TAMMBER`: Massively parallel autonomous MD sampling `github.com/tomswinburne/tammber`
- `QM/ML:` Hybrid DFT/ML-MD simulations `github.com/marseille-matmol/LML-retrain`

Other Interests / Skills

- Native English speaker, advanced French speaker (working language at CNRS)
- Entrepreneurship: founded UK-made rucksack brand, sold worldwide, closed on UK emigration

References

Prof D J Wales FRS, University of Cambridge *(2020-. 2 students, 4 articles)* dw34@cam.ac.uk
Prof Dr. J Neugebauer, Max Planck Dusseldorf *(2020-. 1 student, 2 articles)* neugebauer@mpie.de
Prof Sergei Dudarev, UKAEA *(Postdoc Mentor, 2015- 7 articles)* sergei.dudarev@ukaea.uk
Prof A P Sutton FRS, Imperial College London *(PhD Supervisor, 4 articles)* a.sutton@imperial.ac.uk