Thomas D Swinburne

CNRS Researcher, CINaM, Aix-Marseille Université

thomas.swinburne@cnrs.fr
http://tomswinburne.github.io

Employment

- 10/18-08/25 Chargé de Recherche CNRS, Aix-Marseille University ("Détachement" from 08/25)
- 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 *Concours European. 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"
  Under 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. Amounts exclude salaries of permanent staff)*

- 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 *(supervisor of 2 postdocs, co-supervisor of 2 PhDs + 2 on-going)*

- 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 since 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 since CNRS appointment in 2018 *(* = 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 *(please see teaching statement for detail)* *Whilst CNRS positions are research-only, my enthusiasm for and enjoyment of teaching and mentorship means I actively seek opportunities*

- 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 first/corresponding author

Full list on next page. Total of 45 articles, 4 public preprints, 36 as first / corresponding author
Google scholar 10/10/24: Citations = 1269, h-index = 20

- Parameter uncertainties of imperfect models in the low noise regime
  TDS and D Perez, arXiv:2402.01810v5, to appear in Mach. Learn.: Sci. & Tech.*
- 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

Typically Python/JaX/C++/MPI. Own codes deployed on petascale machines (20k-100kCPUs)

- `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-MD/ML simulations *`github.com/marseille-matmol/LML-retrain`*
- `PyGT`: Python Graph Transformation *(MSc of D Kannan, U Cambridge) `pygt.readthedocs.io`*

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

Publications and preprints in chronological order *(* = first / corresponding author)*

45 articles, 3 preprints, 5 in prep. Corr. author 40/53. Google scholar citations=1222, h-index=20

1. **Theory and simulation of the diffusion of kinks on dislocations in bcc metals* TDS et al., Physical Review B, 2013
2. *Collective transport in the discrete Frenkel-Kontorova model TDS, Physical Review E, 2013
3. *Classical mobility of highly mobile crystal defects TDS et al., Physical review letters, 2014
4. *Thermally-activated non-Schmid glide of screw dislocations in W using atomistically-informed kinetic Monte Carlo simulations* Stukowski et al., International Journal of Plasticity, 2015
5. **Phonon drag force acting on a mobile crystal defect: Full treatment of discreteness and nonlinearity* TDS et al., Physical Review B, 2015
6. *Theory of the deformation of aligned polyethylene* Hammad et al., Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2015
7. **Picosecond dynamics of a shock-driven displacive phase transformation in Zr* TDS et al., Physical Review B, 2016
8. **Fast, vacancy-free climb of prismatic dislocation loops in bcc metals* TDS et al., Scientific reports, 2016
9. *A phenomenological dislocation mobility law for bcc metals* Po et al., Acta Materialia, 2016
10. **Low temperature diffusivity of self-interstitial defects in tungsten* TDS et al., New Journal of Physics, 2017
11. **Computing energy barriers for rare events from hybrid quantum/classical simulations through the* virtual work principle TDS et al., Physical Review B, 2017
12. **Self-optimized construction of transition rate matrices from accelerated atomistic simulations with Bayesian uncertainty quantification* TDS et al., Physical Review Materials, 2018
13. **Kink-limited Orowan strengthening explains the brittle to ductile transition of irradiated and unirradiated bcc metals* TDS et al., Physical Review Materials, 2018
14. *Atomistic-to-continuum description of edge dislocation core: Unification of the Peierls-Nabarro model with linear elasticity* Boleininger et al., Physical Review Materials, 2018
15. **Unsupervised Calculation of Free Energy Barriers in Large Crystalline Systems* TDS et al., Physical Review Letters, 2018
16. *Hybrid quantum/classical study of hydrogen-decorated screw dislocations in tungsten: Ultrafast pipe diffusion, core reconstruction, and effects on glide mechanism* Grigorev et al., Physical Review Materials, 2020
17. *Quantum de-trapping and transport of heavy defects in tungsten* Arakawa et al., Nature Materials, 2020
18. **Defining, calculating, and converging observables of a kinetic transition network* TDS et al., Journal of Chemical Theory and Computation, 2020
19. *Statistical mechanics of kinks on a gliding screw dislocation* Boleininger et al., Physical Review Research, 2020
20. **Machine learning surrogate models for prediction of point defect vibrational entropy* Lapointe et al., Physical Review Materials, 2020
21. *Ultraviolet catastrophe of a fluctuating curved dislocation line* Boleininger et al., Physical Review Research, 2020
22. **Anharmonic free energy of lattice vibrations in fcc crystals from a mean-field bond* TDS et al., Physical Review B, 2020
23. **Rare events and first passage time statistics from the energy landscape* TDS et al., The Journal of Chemical Physics, 2020
24. *A semi-grand canonical kinetic Monte Carlo study of single-walled carbon nanotube growth* Förster et al., AIP Advances, 2021
25. *Femtosecond quantification of void evolution during rapid material failure* Coakley et al., Science advances, 2020
26. **Optimal dimensionality reduction of Markov chains using graph transformation* Kannan et al., The Journal of Chemical Physics, 2020
27. **Automated calculation and convergence of defect transport tensors* TDS et al., npj Computational Materials, 2020
28. *Anharmonic effect on the thermally activated migration of $\{10\bar{1}2\}$ twin interfaces in magnesium* Sato et al., Materials Research Letters, 2021
29. *Piezomagnetic switching and complex phase equilibria in uranium dioxide* Antonio et al., Communications Materials, 2021

30. **Uncertainty and anharmonicity in thermally activated dynamics* TDS, Computational Materials Science, 2021
31. *Interstitialcy-based reordering kinetics of Ni3Al precipitates in irradiated Ni-based super alloys* Ferasat et al., Materialia, 2021
32. *Accelerated molecular dynamics simulations of dislocation climb in nickel* Fey et al., Physical Review Materials, 2021
33. *Efficient and transferable machine learning potentials for the simulation of crystal defects in bcc Fe and W* Goryaeva et al., Physical Review Materials, 2021
34. **Reaction–drift–diffusion models from master equations: application to material defects* TDS et al., Modelling and Simulation in Materials Science and Engineering, 2022
35. *Capabilities and limits of autoencoders for extracting collective variables in atomistic materials science* Baima et al., Physical Chemistry Chemical Physics, 2022
36. **Machine learning surrogate models for strain-dependent vibrational properties and migration rates of point defects* Lapointe et al., Physical Review Materials, 2022
37. **Temperature dependent stacking fault free energy profiles and partial dislocation separation in FCC Cu* Namakian et al., Computational Materials Science, 2023
38. **Calculation of dislocation binding to helium-vacancy defects in tungsten using hybrid ab initio-machine learning methods* Grigorev et al., Acta Materialia, 2023
39. *Nanoindentation of tungsten: From interatomic potentials to dislocation plasticity mechanisms* Domínguez-Gutiérrez et al., Physical Review Materials, 2023
40. **Analysing ill-conditioned Markov chains* Woods et al., Philosophical Transactions of the Royal Society A, 2023
41. *Compact A15 Frank-Kasper nano-phases at the origin of dislocation loops in face-centred cubic metals* Goryaeva et al., Nature Communications, 2023
42. **Temperature dependence of generalized stacking fault free energy profiles and dissociation mechanisms of slip systems in Mg* Namakian et al., Computational Materials Science, 2024
43. **Coarse-Graining and Forecasting Atomic Material Simulations with Descriptors* TDS, Physical Review Letters, 2023
44. **ParSplice: strong exa-scaling of molecular dynamics* TDS, OpenKIM Review, 2024
45. **Sampling-free computation of finite temperature material properties in isochoric and isobaric ensembles using the mean-field anharmonic bond model* Dsouza et al., Physical Review B, 2024
46. **Parameter uncertainties for imperfect surrogate models in the low-noise regime* TDS et al., arXiv preprint arXiv:2402.01810v3, 2024 *(to appear in Machine Learning: Science & Technology)*
47. **Exploring the parameter dependence of atomic minima with implicit differentiation* Maliyov et al., arXiv preprint arXiv:2407.02414, 2024 *(to appear in NPJ Computational Materials)*

Manuscripts under review

48. *A foundation model for atomistic materials chemistry* Batatia *et al.*, arXiv preprint arXiv:2401.00096, 2023 *(under review at Nature)*
49. *Activation entropy of dislocation glide* Allera *et al.* 2024, *(under review at Nat. Communications)*

Manuscripts in late stage of preparation (intended submission in early 2025)

50. **QM/ML simulations of carbon strengthening in tungsten*, Grigorev *et al.,* for submission to PRMat
51. **Material modelling under misspecification* Subamaryam *et al.*, for submission to NPJ Comp. Mat.