Robert Shaw

Department of Chemistry, University of Sheffield, Sheffield S3 7HF, UK
e: r.shaw@sheffield.ac.uk, w: www.rashaw.net

- Creative solutions to mathematical, computational, and theoretical problems in the physical sciences
- Optimisation, machine and deep learning, and the design of efficient data structures and algorithms for faster computational science code

EMPLOYMENT

2021 – Present **Postdoctoral Research Associate in Machine Learning for Basis Set Development**, Department of Chemistry, University of Sheffield, Sheffield, UK

2019 – 2021 **Research Officer in Machine Learning for Materials Discovery,** ARC Centre for Excellence in Exciton Science, RMIT University, Melbourne, Australia

EDUCATION

2016 – 2019 **PhD in Theoretical Chemistry, University of Sheffield**
Passed with no corrections

Supervisor: Dr. J. Grant Hill
Thesis: "Low-scaling correlated methods for intermolecular interactions"
Synopsis: The development and implementation of novel approaches for accurately treating large systems of interacting molecules in the condensed phases.

2015 – 2016 **MSc Theoretical and Computational Chemistry, Theory and Modelling in the Chemical Sciences CDT, University of Oxford, *Distinction***
2015 – 2017 **MSc Mathematics, Open University, *Distinction***
2011 – 2015 **MChem Chemistry, University of Sheffield, *1st class honours***
2010 – 2015 **BSc Mathematics, Open University, *1st class honours***
2003 – 2010 **The Leventhorpe School**
6 A-Levels, A*: Maths, Further Maths, Physics, Chemistry, A: Music, Computing
15 GCSEs (11 A*s, 4 As)

AWARDS, FUNDING AND PUBLICATIONS

- Eleven published papers (list at end), eight as first author, including one as sole author, with a total of 54 citations (as of 10/10/2020).
- Turner Prize for outstanding PhD thesis (2020, Sheffield)
- Coulson Prize for best research talk at an RSC conference (2019, Nottingham)
- Faculty of Science 1st place poster prize for PhD research (2018, Sheffield)
- Helped write successful NVIDIA hardware grant proposal for machine learning in quantum chemistry method developments
- Undergraduate Research Bursary, 2017 (£1600), providing a stipend for an undergraduate student, working on modelling halogen bonds in solution.
- RSC Travel Bursary (£300) covering the costs of attending and presenting at a conference on artificial intelligence in the physical sciences.

- TMCS Prize for best in year (2016, Oxford)
- Haworth Medal for best degree (2015, Sheffield)
- Maitlis Prize for best MChem project (2015, Sheffield)
- OUP and Wharton Prizes for best results (2014/2012, Sheffield)

PROFESSIONAL SKILLS

- Mathematician with strong background in statistics and analysis, in particular as applied to partial differential equations; this has included using machine/deep learning methods, studying the application of neural networks to chemical problems.
- Detailed knowledge of electronic structure theory, particularly the development of mean-field and perturbative methods, and the application of field theories in the condensed phases.
- Extensive programming experience in C/C++, Python, and Fortran.
- Proficiency with data processing, analysis, and visualization using R and Python.
- Lead developer of the Argon app for iOS, Mac, Windows, and Android – therefore experience of cross-platform, app-based development, and UI design
- Creation of, and contribution to, large-scale software projects (see www.github.com/robashaw), including:
    - Named developer on the Psi4 quantum chemistry package;
    - Contributor to Entos QCore and QCSerenity quantum chemistry packages;
    - Creator of libecpint, an open-source, self-generating C++ library for the rapid evaluation of integrals over effective core potentials – up to 100 times faster than traditional approaches;
    - Creator of GAMMA, my own full-featured ab initio quantum chemistry package, specialising in efficient correlated methods for intermolecular interactions;
    - Creator of Knapsack, for the rapid sampling of bosonic configurations in the calculation of photophysical properties.
- Significant experience of modelling physical systems:
    - Developed a linear scaling method for intermolecular interactions based on absolutely localised molecular orbitals with a random-phase approximation correlation treatment; this can accurately treat thousands of molecules on a single desktop computer;
    - Developed algorithms for dimensionality reduction and sampling of vibronic configuration contributions to intramolecular electronic relaxation processes;
    - In collaboration with experimentalists, I have been running molecular dynamics simulations on dye pairs attached to DNA and proteins, with the aim of modelling the electron and energy transfer between them.
- Experience collaborating and communicating across disciplines and institutions, with biophysicists and computer scientists.
- Using and managing high-performance computing facilities, including handling massively parallel architectures and graphical processing units
- Strong technical writing and word processing (LaTeX, MS Word) skills

TEACHING, OUTREACH, AND LEADERSHIP EXPERIENCE

- One of the creators of the Argon app (www.argonmd.co.uk), an educational sandbox for molecular dynamics simulations; this has included presenting it at major scientific festivals, including Cheltenham Science Festival, and at university outreach events.

- Official co-supervisor of two graduate students at RMIT (one PhD and one MSc by research); the MSc by research completed with distinction in September 2020.
- Established and ran tutorials for Sheffield fourth-year computational and theoretical master's students.
- Designed and organised Intro to Python workshops for undergraduate students.
- Tutor on first-year science critical thinking course.
- Supervision of undergraduate project students.
- Primary supervision of a summer placement student.
- Teaching assistant at the 2016 UK Theoretical Chemistry summer school at Oxford.
- Private tutor in science, mathematics, and music.
- Initiated and organised weekly meetings of the theoretical groups at Sheffield, and the running of tutorial sessions for the undergraduate project students.
- Helped organise the Midlands Computational Chemistry and Royal Society of Chemistry Theoretical Chemistry Group meetings in 2017/18.

EQUALITY, DIVERSITY, AND INCLUSION

I am currently a trustee of Pride in STEM, an organisation that advocates for LGBTQ+ scientists. I am also currently on the ARC Centre for Excellence in Exciton Science EDI committee. Work to improve EDI in science is something I am very passionate about, and forms a key part of my professional life.

PROFESSIONAL SOCIETIES

Associate member of the Royal Society of Chemistry (2017 – Present)
Associate member of the London Mathematical Society (2016 – Present)
Associate Fellow of the HEA (2019)

INTERESTS

I have performed as a musician both in groups and independently for the past 15 years. I am particularly interested in composition, working on open-source projects developing audio production tools, including using neural networks to learn composition styles. I also have recently been involved in organising events advocating for the LGBT community.

PUBLICATION LIST

R. A. Shaw and J. G. Hill, "Libecpint: a C++ library for the efficient evaluation of integrals over effective core potentials", Journal of Open Source Software, 2021, **6**(60), 3039

R. A. Shaw, A. Manian, I. Lyskov and S. P. Russo, "Efficient enumeration of bosonic configurations with applications to the calculation of non-radiative rates", Journal of Chemical Physics, 2021, **154**(8), 084102

R. A. Shaw, T. Johnston-Wood, B. Ambrose, T. D. Craggs and J. G. Hill, "CHARMM-DYES: Parameterization of fluorescent dyes for use with the CHARMM force field", Journal of Chemical Theory and Computation, 2020, **16**(12), 7817

T. J. Hughes, **R. A. Shaw** and S. P. Russo, "Computational investigations of dispersion interactions between small molecules and graphene-like flakes", Journal of Physical Chemistry A, 2020, **124**(46), 9552

R. A. Shaw, “The completeness properties of Gaussian-type orbitals in quantum chemistry”, International Journal of Quantum Chemistry, 2020, **120**(17), e26264

D. Smith et al., “Psi4 1.4: Open-Source Software for High-Throughput Quantum Chemistry”, Journal of Chemical Physics, 2020, **152**(18), 184108

B. Ambrose, M. Willmott, T. Johnston-Wood, **R. A. Shaw,** J. G. Hill, T. D. Craggs, “Below the FRET limit”, Biophysical Journal, 2020, **118**(3), 615as

R. A. Shaw and J. G. Hill, “A linear-scaling method for non-covalent interactions: An efficient combination of absolutely localized molecular orbitals and a local random phase approximation approach”, Journal of Chemical Theory and Computation, 2019, **15**(10), 5352-5369

R. A. Shaw and J. G. Hill, “A simple model for halogen bonds”, Inorganics, 2019, **7**(19)

R. A. Shaw and J. G. Hill, “Midbond basis functions for weakly bound complexes”, Molecular Physics, 2018, **116**(11), 1460-1470

S. K. Singh, P. R. Joshi, **R. A. Shaw,** J. G. Hill and A. Das, “Interplay between n→ π* interaction and hydrogen bond in an analgesic drug salicin”, Physical Chemistry Chemical Physics, 2018, **20**, 18361-18373

R. A. Shaw and J. G. Hill, “Prescreening and efficiency in the evaluation of integrals over ab initio effective core potentials”, Journal of Chemical Physics, 2017, **147**(7), 074108

R. A. Shaw and J. G. Hill, “Approaching the Hartree-Fock Limit through the Complementary Auxiliary Basis Set Singles Correction and Auxiliary Basis Sets”, Journal of Chemical Theory and Computation, 2017, **13**, 1691-1698

R. A. Shaw, J. G. Hill and A. C. Legon,“Halogen Bonding with Phosphine: Evidence for Mulliken Inner Complexes and the Importance of Relaxation Energy”, Journal of Physical Chemistry A, 2016, **120**, 8461-8468