

Adam Baskerville

Curriculum Vitae

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I am currently undertaking a Ph.D. in quantum chemical physics at the University of Sussex under the supervision of Dr Hazel Cox. My research interests include atomic and molecular physics, chemical physics, quantum mechanics, theoretical physics and scientific computing.

Education

Ph.D., Department of Chemistry, School of Life Sciences, University of Sussex, UK Sept 2014-Present

Ph.D. in quantum chemical physics. My research involves using a very accurate series solution method to solve the all-particle Schrödinger equation for three-particle systems in order to obtain accurate energies and wavefunctions. My work has included studying nuclear motion in molecular systems, manifestations of Coulomb holes in three-particle atomic systems, investigation into the atomic to molecular transition and studying the radial and angular properties of atoms and molecules. Expected thesis submission date: March 28th 2018.

MPhys, Department of Physics, School of Physical Sciences, University of Kent, UK Sept 2010-2014

Master of Physics and Astrophysics, First-class honours. Modules undertaken include relativity, optics and Maxwell's equations, advanced quantum physics, particle physics, condensed matter physics, astrophysics and cosmology, physics problem solving and advanced mathematical physics. For my final year project I conducted research into the manifestation of magnetic monopole pseudo-particles in a substance known as spin ice using semi-classical physics, with emphasis on terbium titanate. I studied if it was possible for electrons contained in a two dimensional electron gas to form bound states within the magnetic fields of the monopoles, and proposed an experiment to form bound states using a nano-scale ferromagnetic needle.

Awards and funding

Talk prize, Young Modellers Forum (YMF) Nov 2017

Awarded for my talk "Going beyond standard approximations in quantum chemistry."

Doctoral overseas grant award, School of Life Sciences, University of Sussex June 2016

Awarded £1000 by the University of Sussex to attend the IX Congress of the International Society for Theoretical Chemical Physics (ISTCP) which took place in North Dakota USA. I presented a poster on my research into nuclear motion in three-particle diatomics and the transition from atomic to molecular systems.

Institute of Physics funding award, Institute of Physics (IOP) April 2016

Awarded £300 to attend the IX Congress of the International Society for Theoretical Chemical Physics (ISTCP) detailed above.

MPhys final year research prize, School of Physical Sciences, The University of Kent July 2014

Awarded for the best final year research project.

Second year student prize, School of Physical Sciences, The University of Kent July 2012

Awarded for the highest total mark in second year.

Teaching experience

Research Supervision, School of Life Sciences, The University of Sussex, UK 2015-Present

Day to day supervision of MChem project students in the Cox group.

Associate Tutor, School of Life Sciences, The University of Sussex, UK 2014-Present

During my PhD studies I assist in teaching mathematics to biosciences foundation year students, data analysis and point group symmetry to first year chemistry students, and computational chemistry to third year chemistry students. This involves demonstrating in problem based workshops and marking.

Student Mentor, School of Physical Sciences, University of Kent, UK 2013-2014

In my final year of my master's degree I was a student mentor and assisted students in the lower years in several modules including Relativity, Optics and Maxwell's equations, Cosmology and advanced mathematical physics. This involved revision of the content they covered in lectures and advising with problem sets.

Conference presentations

Talk: "Going beyond standard approximations in quantum chemistry", Young Modellers Nov 2017

Forum, Greenwich, UK

Talk: "Excited S states of two electron atoms", Quantum Physics and Quantum Technology, Sept 2017

Berlin, Germany

- Poster:** "Quantum effects of particle motion in atomic and molecular three-particle systems", Life Sciences Research Symposium, University of Sussex, UK Sept 2016
- Poster:** "Quantum effects of particle motion in atomic and molecular three-particle systems", IX Congress of the International Society for Theoretical Chemical Physics, North Dakota, USA July 2016
- Poster:** "Intracule and centre of mass particle densities for atomic and molecular three-particle systems", IMAMPC conference, Birmingham, UK August 2015
- Session Chair:** General theory session, IMAMPC conference, Birmingham, UK August 2015
- Poster:** "Magnetic monopoles in spin ice", Gyorffy-SuperMagCorrelation meeting, Bristol, UK Sept 2014
- Oral Presentation:** "Magnetic monopoles in spin ice", Physical sciences research symposium, University of Kent, UK May 2014

Transferable skills training

MapleSoft training course, Institute of Physics (IOP) March 2016

I took part in a training course sponsored by MapleSoft titled "*Applying the power of computer algebra to theoretical physics.*" They covered various applications of Maple in theoretical calculations, and showcased new software features.

Virtual winter school for computational chemistry February 2016

This online conference hosted talks along with interactive question and answer sessions, on a variety of subjects from computational solid state physics and chemistry, to molecular excited state calculations and inclusion of relativistic corrections.

NSCCS workshop, Imperial College London September 2014

I took part in a workshop organised by the EPSRC UK National Service for Computational Chemistry Software (NSCCS) to learn and use the Gaussian09 software package.

Computer skills

I am competent in the following programming languages: C++, Python, Bash, Maple, Mathematica, \LaTeX .

C++ and Python were used for developing matrix eigenvalue solvers, numerical integration, spline fitting and a variety of other applications. Bash scripts were written to act as a bridge between the larger C++ and Python codes along with automation of a large number of data analysis tasks. Maple and Mathematica were used for symbolic calculations, such as analytical integration and simplifying large expressions.

Publications

- [1] Quantum effects of nuclear motion in three-particle diatomic ions
Baskerville, A. L., A. W. King and Cox, H.
Phys. Rev. A 94 (2016) 042512-1–042512-9. doi: [10.1103/PhysRevA.94.042512](https://doi.org/10.1103/PhysRevA.94.042512)
- [2] Hartree-Fock implementation using a Laguerre-based wavefunction for the ground-state and correlation energies of two-electron atoms
King, A. W., Baskerville, A. L. and Cox, H.
Philos. T. R. SOC. A 376 (2017) p. 20170153. doi: [10.1098/rsta.2017.0153](https://doi.org/10.1098/rsta.2017.0153)
- [3] The Series Solution Method in Quantum Chemistry for Three-Particle Systems
Cox, H. and Baskerville, A. L.
Adv. Quant. Chem. (Accepted)

Personal interests

I enjoy strongman and powerlifting which involves strenuous training and dedication. I enjoy astronomy and astrophotography along with programming Raspberry Pi boards to complete various tasks.

References

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