ALEX G. SQUIRES

(+44) 7732585206 | a.g.squires@bath.ac.uk

EDUCATION

Doctorate — University of Bath

2017-present *Ph.D.* - Computational modelling of defects in battery materials

First Degree — University College London

2013-2017 *Chemistry MSci.* - First Class Honours

- *Research Project*, Computational screening of bismuth oxyhalides for photocatalysis
- *Dissertaion*, The prospects for *p*-type transparent conducting oxides

PUBLICATIONS

① A. G. Squires, D. O. Scanlon, B. J. Morgan, Native Defect Chemistry of Lithium Conducting Garnets, Chem. Mater. 2020, 32, 5, 1876–1886

GRANTS AND AWARDS

① *Early Career Researcher Award* - Science and Technology Facilities Council

② *Armourers and Brasier's Society Travel Grant*

③ *University of Bath Doctoral College Placement Support Fund*

④ *The Roy Prize* - Royal Society of Chemistry Solid State Group

SELECTED PRESENTATIONS

① *Contributed*, "Intrinsic defect chemistry of lithium conducting garnets", Royal Society of Solid State Chemistry Group Christmas Meeting 2018—**Best presentation award**

② *Contributed*, "Computational modelling of the defective and electronic properties of lithium conducting garnets", MRS Fall Meeting 2019

③ *Contributed*, "Native defects and their doping response in the lithium conducting garnet $Li_7La_3Zr_2O_{12}$", MC14 2019

④ *Invited*, "First principles modelling of electronic and defective properties of $Li_7La_3Zr_2O_{12}$, seminar, Yonsei University

⑤ *Invited*, "Ordering in sodium cathode material Na_2RuO_3 for capacity and stability", seminar, University of California Santa Barbara

TEACHING EXPERIENCE

2019-present *Ph.D. Tutor*, The Brilliant Club
Teaching a course based around my research to secondary school students, to expose them to university style learning.

2017-present *Graduate Teaching Assistant*, University of Bath
Demonstration in computational chemistry labs at the University of Bath, ensuring the undergraduates have grasped the key concepts and acting as an approachable source of support.

2014-2016 *Personal Tutor*
Tutoring in A level Chemistry, AS Physics and GCSE maths and sciences. Covering all ranges of exam board syllabuses ensuring the students can achieve and exceed their targeted grades.

2014-2015 *Transition Mentor*, UCL
Helping first year students adapt to university life both academically and non-academically. Leading weekly sessions covering concepts they have been struggling with. Helping them deal with any personal or administrative issues that might come up in their first term at UCL.

RELEVANT SKILLS

PROGRAMMING – proficient with **Python**, familiar with **Julia**.

DFT – proficient with **VASP**, familiar with **Crystal**.

MISCELLANEOUS SCIENTIFIC CODES USED – **CASM, CLEASE, icet** (cluster expansion), **ASE, pymatgen** (pre and post processing DFT calculations), **CPLAP, SC-FERMI** (point defect analysis).

GENERAL COMPUTATIONAL SKILLS - proficient with LaTeX, comfortable with Windows, Linux, and Mac OS.

REFEREES

Dr Benjamin Morgan
Royal Society University Research Fellow,
Department of Chemistry,
University of Bath,
Bath,
BA2 7AX.
b.j.morgan@bath.ac.uk

Prof. David Scanlon
Chair of Computational Materials Design,
Department of Chemistry,
University College London,
20 Gordon Street,
London,
WC1H 0AJ.
d.scanlon@ucl.ac.uk