

# Rhys Edward Andrew Goodall

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<b>EDUCATION</b>	<b>PhD - Physics</b> 2018 - 2022 Jesus College, University of Cambridge
	<b>MSci - Experimental and Theoretical Physics</b> 2017 - 2018 Robinson College, University of Cambridge
	<b>BA - Natural Sciences</b> 2014 - 2017 Robinson College, University of Cambridge

<b>EXPERIENCE</b>	<b>Machine Learning Scientist (Internship)</b> April 2022 - Present Chemix.ai, San Francisco Bay Area, USA <ul style="list-style-type: none"><li>Implemented deep learning-based pipeline for chemical formulation design that scales more efficiently than shallow models on large experimental data sets enabled by high-throughput experimentation platform.</li></ul>
	<b>Machine Learning Scientist (Internship)</b> Jan 2022 - Mar 2022 Mat3ra.com, San Francisco Bay Area, USA <ul style="list-style-type: none"><li>Extended cloud-based high performance compute platform to incorporate material science specific machine learning tools including <code>SISSO</code> and <code>DeePMD-Kit</code>.</li></ul>
	<b>Graduate Student Researcher</b> Oct 2019 - Jan 2022 Department of Physics, University of Cambridge, UK <ul style="list-style-type: none"><li>Conceptualized the <code>roost</code> and <code>wren</code> frameworks for machine learning guided materials discovery that led to 50% lower errors for composition-based screening and 3x improvement in efficiency for prototyping-based workflows respectively.</li><li>Developed and open sourced <code>aviary</code> and <code>pymatvis</code> python packages and contributed additional analysis functionality to <code>pymatgen</code> to enable all results to be independently reproducible.</li></ul>
	<b>Undergraduate Supervisor</b> Jan 2019 - June 2020 Department of Physics, University of Cambridge, UK <ul style="list-style-type: none"><li>Teaching assistant for Quantum Condensed Matter Physics and Computational Physics classes for final year undergraduate students.</li><li>Supervised masters student working on the application of machine learning to the prediction of major products in inorganic reactions resulting in a publication in Chemistry of Materials.</li></ul>
	<b>Resident Fellow</b> Sep 2019 - Dec 2019 Institute for Pure & Applied Mathematics, UCLA, USA <ul style="list-style-type: none"><li>Resident fellow for the 'Machine Learning for Physics and the Physics of Learning' Long Program.</li><li>Chaired research group looking at uncertainty estimation, calibration and active learning using machine learning models with a focus on applications in Material Science.</li></ul>
	<b>EnterpriseTech Team Leader</b> Jan - May 2018 Judge Business School, University of Cambridge, UK <ul style="list-style-type: none"><li>Led a team of five in assessing the potential commercialisation of an early-stage nanotechnology product for the functionalisation of nanoparticles.</li></ul>

<b>SKILLS</b>	<b>Software Engineering</b> - Python, Git, Conda, Slurm
	<b>Machine Learning</b> - PyTorch, PyG, BoTorch, Scikit-Learn, Keras
	<b>Numerical Analysis</b> - Pandas, Numpy, Scipy
	<b>Visualisation</b> - Matplotlib, Plotly, Inkscape, Jupyter, LaTeX

<b>AWARDS &amp; PRIZES</b>	<b>BatteryDev Hackathon (First Place)</b>	2022
	Member of winning team for the QuantumScape EIS challenge at BatteryDev Hackathon 2022.	
	<b>Institute of Pure &amp; Applied Mathematics Research Fellowship</b>	2019
	Full award covering expenses for Long Program at the Institute for Pure & Applied Mathematics, UCLA.	
	<b>Cavendish Laboratory Departmental Studentship</b>	2018
	Full studentship awarded for PhD study at the Cavendish Laboratory.	
	<b>Cavendish Laboratory Microsoft Research Prize</b>	2018
Cavendish Laboratory Prize for the most novel results in a Masters level Computational Research Project.		
<b>Robinson College Mathers' Prize</b>	2018	
College prize awarded to the graduating student obtaining the best examination results in the Natural Sciences at the College.		
<b>NERC Research Experience Placement Grant</b>	2017	
Natural Environment Research Council grant awarded for interdisciplinary research within the Environmental Sciences.		
<b>RSC Bill Bryson Prize (Highly Commended)</b>	2014	
Royal Society of Chemistry prize in recognition of efforts in service of scientific communication and engagement.		

**PUBLICATIONS** Goodall, R. E. A., Lee, A. A. Predicting Materials Properties Without Crystal Structure: Deep Representation Learning From Stoichiometry. *Nature Communications* (2020) 11 (1), 1-9.

Malik, S. A., Goodall, R. E. A., Lee, A. A. Predicting the Outcomes of Inorganic Reactions With Deep Learning. *Chem. Mater.* (2021) 33, 2, 616624.

Goodall, R. E. A., Lee, A. A. Data-Driven Approximations to the Bridge Function Yield Improved Closures for the Ornstein-Zernike Equation. *Soft Matter* (2021) 17 (21), 5393-5400.

Goodall, R. E. A., Zhu, B., MacManus-Driscoll, J. L., Lee, A. A. Materials Informatics Reveals Unexplored Structure Space in Cuprate Superconductors. *Advanced Functional Materials* (2021) 2104696.

Goodall, R. E. A., Parackal, A. S., Faber, F. A., Armiento, R., Lee, A. A. Rapid Discovery of Stable Materials by Coordinate-free Coarse Graining. *Science Advances* (2022) 8, eabn4117.

**WORKSHOPS & PREPRINTS** Goodall, R. E. A., Lee, A. A. Inference of a Universal Ornstein-Zernike Closure Relationship with Machine Learning. *NeurIPS 2019 Workshop on Machine Learning and the Physical Sciences*.

Goodall, R. E. A., Parackal, A. S., Faber, F. A., Armiento, R., Lee, A. A. Wyckoff Set Regression for Materials Discovery. *NeurIPS 2020 Workshop on Machine Learning and the Physical Sciences*.

**ACTIVITIES** Water Polo (Cambridge University Varsity Team, West London Penguin).  
Volunteering (London 2012 Games Maker, Science Mentor).  
Student Leadership (President - Robinson College Students' Association (RCSA) 2016-2017, Treasurer - Jesus College Middle Combination Room (MCR) 2020-2021)