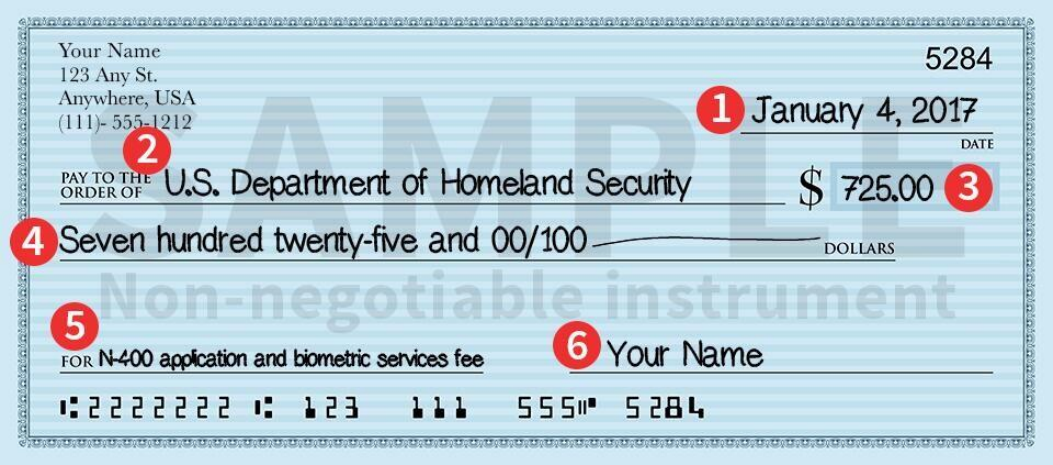

Attach checks with clipper. Always check the USCIS website for the most recent fees! See check writing instructions: https://www.uscis.gov/forms/filing-fees

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Initial Evidence in Support of the I-140 Immigrant Petition

Petitioner and Beneficiary:	Ryan-Rhys Griffiths
Classification Sought:	Employment-Based Immigration, First Preference Extraordinary Ability in Science (EB-1A). Sec. 203(b)(1) INA [8 U.S.C. 1153].

To whom it may concern,

This letter is respectfully submitted in support of the petition of Dr. Ryan-Rhys Griffiths for classification as a qualified immigrant under the first preference employment immigration for Aliens of Extraordinary Ability pursuant to section 203(b)(1)(A) of the Immigration and Nationality Act ("the Act"). This evidence shows that Dr. Griffiths is an alien of extraordinary ability in the sciences, specifically in Machine Learning and the Natural Sciences, who has sustained national and international acclaim with his achievements recognized in the field of expertise. More precisely, this letter provides evidence that:

1. Dr. Griffiths satisfies four of ten criteria listed in 8 CFR, Section 204.5(h)(3), namely:
    - Dr. Griffiths has made original scientific and scholarly contributions of major significance in the field of Machine Learning and the Natural Sciences. (section 2.1)
    - Dr. Griffiths's authorship of scholarly articles in the field in professional or major trade publications or other major media. (section 2.2)
    - Participation of Dr. Griffiths as a judge of the work of others in the field (section 2.3)
    - Published material about Dr. Griffiths in professional or major trade publications or other major media, relating to Dr. Griffiths's work in the field (section 2.4)
2. Dr. Griffiths reached a level of expertise indicating that he is one of that small percentage who have risen to the very top of the field of Machine Learning and the Natural Sciences – section 3.1.
3. Dr. Griffiths sustained national or international acclaim and that his achievements have been recognized in the field of Machine Learning and the Natural Sciences – section 3.2.

Pursuant to 8 CFR, Section 204.5(h)(1), Dr. Griffiths may file an I-140 visa petition for classification under Section 203(b)(1)(A) of the Act as an alien of extraordinary ability in the sciences on his own behalf.

Pursuant to 8 CFR, Section 204.5(h)(5), neither an offer for employment in the United States nor a labor certification is required for this classification.

1 Summary of Dr. Griffiths's achievements and qualifications

Dr. Griffiths is a Postdoctoral Research Scientist in the Adaptive Experimentation team at Meta Research, Menlo Park, California [Exhibit 44]. Dr. Griffiths joined Meta Research in August 2022 after completing his PhD from the University of Cambridge in the United Kingdom (UK). His research focusses on Machine Learning and the Natural Sciences. Before coming to the US, Dr. Griffiths lived in the UK for 10 years, completing his undergraduate studies at Imperial College London, and his masters and PhD degrees at the University of Cambridge, two leading universities worldwide [Exhibit 1] [Exhibit 43]. Dr. Griffiths graduated with First Class Honours in Chemistry with Molecular Physics from Imperial College London [Exhibit 43].

Dr. Griffiths works on machine learning methodologies, namely Gaussian processes and Bayesian optimization as well as applications of machine learning in the natural sciences. Bayesian optimization is currently utilized across many areas of artificial intelligence (AI) as a state-of-the-art hyperparameter optimizer for machine learning algorithms making the deployment of AI solutions both cheaper and faster. Bayesian optimization is also a core methodology for accelerating the discovery of novel materials and molecules in areas such as drug discovery and renewable energy. Dr. Griffiths has worked for over 6 years on improving Bayesian optimization methodology to achieve speedups and cost-savings for AI algorithms as well as for the discovery of novel molecular and chemical materials.

Dr. Griffiths has made major contributions to the field of machine learning and the natural sciences. He was the lead author on one of the first papers to leverage generative AI for drug molecule generation, a field which promises to accelerate the discovery of therapeutics for conditions including cancer, Parkinson's disease, and diabetes (section 2.1.1). He has also coauthored Heteroscedastic Evolutionary Bayesian Optimisation (HEBO), a state-of-the-art machine learning algorithm that won the 2020 NeurIPS Black-box optimization challenge, a competition sponsored by Meta and Twitter at NeurIPS, the world's premier machine learning conference. HEBO has subsequently been used by the ATLAS experiment group at the Large Hadron Collider in CERN (section 2.1.2). Dr. Griffiths has also leveraged machine learning directly to discover novel photoswitch molecules, a class of compound with applications as agents for vision restoration in the blind, as anti-cancer therapeutics, as well as for environmental applications in renewable energy (section 2.1.3). More recently, Dr. Griffiths has coauthored a paper which analyzes the mathematical capabilities of ChatGPT that has acquired 194 citations this year alone (section 2.1.4).

To date, Dr. Griffiths has published over 20 peer-reviewed scientific articles (7 as lead author) that have been featured in top journals in the machine learning and science fields. The articles Dr. Griffiths authored have accrued 1042 citations as of November 2023 and have been cited more than 500 times in the past 11 months, showing a marked increase in the impact of his research. Additionally, Dr. Griffiths's papers have accrued significantly more citations than the articles of his peers (section 2.2.3).

Dr. Griffiths has been active as a judge of the work of others having conducted 49 peer reviews in 23 leading journals in the field of Machine Learning and the Natural Sciences (section 2.3).

Dr. Griffiths's research has received significant media attention. He maintains 18,000+ followers on LinkedIn and 4,000+ followers on Twitter. His paper on the mathematical capabilities of ChatGPT was featured in Synced, a leading online AI technology and industry review outlet (section 2.4.1). His GAUCHE and FlowMO software libraries have been used in industry by the AstraZeneca AI group and Relay Therapeutics, an American biotechnology company. (section 2.4.3).

As evidenced by six recommendation letters from distinguished professors and managers in the machine learning industry, his 20+ scientific publications, 49 peer-reviews, Dr. Griffiths has risen to the top of the field of Machine Learning and the Natural Sciences (section 3.1). Dr. Griffiths has further sustained this performance as evidenced by the increasing number of citations he has recently obtained (500+ in the past 11 months alone).

2 Proof of Dr. Griffiths's Extraordinary Ability

2.1 Evidence of original scientific, scholarly, artistic, athletic, or business-related contributions of major significance to the field

2.1.1 Evidence of original scientific contribution: One of the first papers using generative AI to propose novel drug molecules

Dr. Griffiths introduced one of the first algorithms to apply generative AI, namely variational autoencoders, to the targeted generation of novel drug molecules which will accelerate the adoption of new and effective medical treatments. At the time of publishing in 2017, Dr. Griffiths's algorithm represented the state-of-the-art in machine-learning based molecule generation. While in 2023, it is no longer the state-of-the-art algorithm, it has catalyzed advances in molecule generation methods as evidenced by 334 citations following its publication in the Chemical Science journal, the flagship journal of the Royal Society of Chemistry [Exhibit 2, Exhibit 9].

"*To provide more specifics on the details of Dr. Griffiths's research, I will begin by discussing his work on "Constrained Bayesian Optimization for Automatic Chemical Design using Variational Autoencoders". In this work Dr. Griffiths improved a system for extending Bayesian optimization to high-dimensional and structured input spaces by using a variational autoencoder (VAE), a deep learning methodology that facilitates transformation of discrete variables such as graphs, strings, and bit vectors to a continuous latent representation. Dr. Griffiths's methodological contribution in this paper was to first highlight a problem in existing VAE- based Bayesian optimization architectures, namely the mismatch between the objectives of the Bayesian optimization Gaussian processes surrogate and the training set support of the VAE. The crux of this problem is that there is a tendency for the Bayesian optimization scheme to select points that lie far away from the support of the VAE training distribution yielding invalid outputs. In his paper, Dr. Griffiths implemented a constraint scheme which increased the number of valid outputs from the model, yielding state-of-the-art performance at the time of its introduction.*"

Prof. XYZ, Professor of XYZ, University of XYZ)

"*Dr. Griffiths has provided many core research contributions within the field of Bayesian optimization. With his paper, "Constrained Bayesian optimization for Automatic Chemical Design using Variational Autoencoders", published in Chemical Science, Griffiths improved on the incumbent state-of-the-art in machine learning-based molecular property optimization. This paper also represented a fundamental advance in Bayesian optimization methodology. Scaling Bayesian optimization to high-dimensional problems has traditionally been a challenging research problem. In his paper, Dr. Griffiths successfully applies variational autoencoders as a tool to reduce the dimensionality of the optimization space facilitating efficient search for novel molecules. Dr. Griffiths's core contribution in this regard was to implement a probabilistic constraint scheme that addressed the problem of invalid generation from the latent space of the variational autoencoder yielding significant performance gains compared to previous algorithms. To date, Dr. Griffiths has received over 260 citations for this contribution alone.*"

Prof. XYZ, Professor of XYZ, University of XYZ)

2.1.2 Evidence of original scientific contribution: Coauthored HEBO, the winning algorithm in the 2020 NeurIPS black-box optimization competition

Dr. Griffiths coauthored the Heteroscedastic Evolutionary Bayesian Optimization (HEBO) algorithm which achieved 1st place at the 2020 NeurIPS black-box optimization competition sponsored by Twitter and Meta, a competition organized at the world's premier machine learning conference. The algorithm was awarded a $6,000 prize for winning the challenge (https://bbochallenge.com/leaderboard/). To this day, HEBO remains a state-of-the-art algorithm for machine learning hyperparameter tuning and has been used earlier this year by the ATLAS experiment at the Large Hadron Collider in CERN (section 2.4.4). It is heavily used in research and industry as evidenced by 1,900+ stars on GitHub (`https://github.com/huawei-noah/HEBO`) as well as 115 citations as of November 2023. It was published in the prestigious Journal of Artificial Intelligence Research in 2022. [Exhibit 29]. The algorithm has subsequently been used as a benchmark algorithm for machine learning-based antibody design against the SARS-CoV (COVID) antigen:

- Khan, A., Cowen-Rivers, A.I., Grosnit, A., Robert, P.A., Greiff, V., Smorodina, E., Rawat, P., Akbar, R., Dreczkowski, K., Tutunov, R. and Bou-Ammar, D., Toward real-world automated antibody design with combinatorial Bayesian optimization. Cell Reports Methods, p.100374, 2023.

and as a hyperparameter optimization algorithm for robotics amongst other applications:

- Liu, P., Tateo, D., Bou-Ammar, H. and Peters, J., Efficient and reactive planning for high speed robot air hockey. In 2021 IEEE/RSJ International Conference on Intelligent Robots and Systems (IROS) (pp. 586-593). 2021.

Further details on the HEBO algorithm are provided by Dr. XYZ and Prof. XYZ:

"*Ryan-Rhys Griffiths's second work is related to the Heteroscedastic Evolutionary Bayesian Optimization (HEBO) algorithm. This algorithm won the 2020 NeurIPS Black- Box Optimization Competition. The*

NeurIPS conference is the top international venue for machine learning research. The HEBO algorithm currently has 115 citations and has been published in the prestigious Journal of Artificial Intelligence Research. The algorithm showed the strongest performance on machine learning hyperparameter tuning tasks in the competition by introducing novel methods for considering heteroscedasticity and non-stationarity of the underlying data via input warping using a Beta Kumaraswamy distribution function and Yeo-Johnson and Box-Cox transforms to correct for heteroscedasticity."

(Prof. XYZ, Professor of XYZ, University of XYZ)

"*Dr. Griffiths has gone on to achieve notable international success in his research. For instance, he jointly developed the heteroscedastic evolutionary Bayesian optimisation (HEBO) algorithm that won the 2020 NeurIPS Competition on Black-Box Optimisation. The HEBO algorithm has subsequently been used notably in the ATLAS experiments at the Large Hadron Collider at CERN.*"

(Prof. XYZ, Professor of XYZ, University of XYZ)

2.1.3 Evidence of original scientific contribution: Lead author on a series of papers using Gaussian processes to discover novel photoswitch molecules

Dr. Griffiths was lead author on the paper, "Data-driven discovery of molecular photoswitches using multi output Gaussian processes. In this work, Dr. Griffiths used a machine learning algorithm based on multioutput Gaussian processes with a Tanimoto kernel to identify a promising photoswitch molecule. The paper was published in Chemical Science, the flagship journal of the Royal Society of Chemistry and was featured as one of the most popular physical and theoretical chemistry articles of 2022 [Exhibit 37]. The collection is described as follows, "This specially curated collection pulls together some of the most popular articles from 2022 in the field of physical and theoretical chemistry. The collection presents some outstanding contributions to the field, ranging from deep learning models for predicting drug-target interactions, through to investigations into colour-tunable persistent luminescence in low-dimensional zinc-organic halide microcrystals." [Exhibit 37]. The paper has acquired 34 citations to date. Dr. Griffiths has additionally made his methodology freely available as the open-source FlowMO and GAUCHE libraries to be used by researchers in academia and in industry. His paper FlowMO was awarded a spotlight contributed talk at the 2020 NeurIPS workshop on machine learning for molecules i.e. it was ranked in the top 5% of accepted papers: `https://neurips.cc/virtual/2020/protected/workshop_16136.html`. His FlowMO software library has subsequently been used by the AstraZeneca AI group (section 2.4.4) as well as Relay Therapeutics (section 2.4.3), a US biotechnology company [Exhibit 42]. His GAUCHE software library was accepted at NeurIPS 2023 [Exhibit 34], the world's premier international machine learning conference [Exhibit 2]: `https://neurips.cc/virtual/2023/poster/70081`

"*I first noticed Dr. Griffiths's work in 2019 when working on Bayesian set optimization and discovering his excellent work around using the Tanimoto kernel in the context of molecular chemistry. Looking at*

his then already substantial track-record and impact, I also realized with amazement that he was still at an early stage of his career (then a PhD student at Cambridge) and upon our discussions online and in [insert placename] I was stunned by his rare computational intelligence and scientific versatility. I must also say that with two of my students we studied and reproduced some of his work, and despite our efforts to find a better approach we ended up corroborating his conclusions and further showing some advantages of the kernel he used in terms of the associated prediction uncertainty."

(Prof. XYZ, Professor of XYZ, University of XYZ)

"*The contribution of GAUCHE is to make available the Gaussian process framework to operate on spaces of molecules, chemical reactions, and proteins. The library is the first to make available modern machine learning frameworks such as PyTorch and Tensorflow (and GPU-based computation) to Gaussian process-based molecular property prediction. The library has already received international attention from the machine learning community with a spotlight (top 5% of accepted papers) at the 2020 NeurIPS Workshop on Machine Learning for Molecules for the paper "Molecular Property Prediction with FlowMO" and has even seen usage in the industry which is rare on such a short timeframe.* "

Prof. XYZ, Professor of XYZ, University of XYZ)

"*Dr. Griffiths released a number of open-source software packages during his PhD, the most notable of which have been the GAUCHE and FlowMO libraries which are currently being used internationally for research in machine learning for chemistry and chemical reaction optimization, as well as in the pharmaceutical industry. The libraries combined have over 100 GitHub stars.*"

(Prof. XYZ, Professor of XYZ, University of XYZ)

"*The FlowMO paper was awarded a spotlight at the 2020 NeurIPS Workshop on Machine Learning for Molecules, a major international venue for discussions on machine learning applied to the molecular sciences. In detail, the FlowMO and GAUCHE software libraries extend Gaussian processes to operate on molecular representations. The particular focus of the work is on commonly-used representations for molecules such as SMILES strings, binary vectors, and graphs. The open-source software implementations are the first to support graphics processing unit (GPU) based machine learning on molecules using Gaussian processes in a modern machine learning framework. The aforementioned considerations are key to making these technologies available to practitioners. So far, in spite of its recency, Dr. Griffiths's research has seen significant uptake in industry with users of GAUCHE including AstraZeneca and Relay Therapeutics.*"

(Prof. XYZ, Professor of XYZ, University of XYZ)

2.1.4 Evidence of original scientific contribution: Coauthored a paper on the mathematical capabilities of ChatGPT.

Dr. Griffiths coauthored a paper that critically analyzed the mathematical capabilities of ChatGPT. To date the paper has accrued 194 citations in the past year alone [Exhibit 2] and has attracted media attention, being featured in Synced, China's leading machine learning periodical. [Exhibit 42]. The paper has recently been accepted to NeurIPS 2023 [Exhibit 34], the world's premier international machine learning conference [Exhibit 2]: `https://neurips.cc/virtual/2023/poster/73421`

"*Dr. Griffiths recently coauthored a paper analyzing the mathematical capabilities of ChatGPT. This paper concluded that ChatGPT did not possess the skills of a graduate level mathematician based on a series of tasks involving proof completion, symbolic integration, and performance assessment as a mathematical search engine. The paper has already received 6 citations in the past month and will serve an important purpose in highlighting some of the limitations of ChatGPT for prospective deployment in the education system.*"

Prof. XYZ, Professor of XYZ, University of XYZ)

2.2 Evidence of authorship of scholarly articles in professional or major trade publications or other major media

2.2.1 Dr. Griffiths has published 23 scientific articles in the field of machine learning and the natural sciences

As evidenced in Dr. Griffiths's Curriculum Vitae [Exhibit 1] and in his Google Scholar profile [Exhibit 2], Dr. Griffiths has so far authored 23 scientific articles (7 as lead author), which have together gathered 1042 citations [Exhibit 2] as of November 2023. Dr. Griffiths's publications are presented in [Exhibit 9] through [Exhibit 33].

2.2.2 Dr. Griffiths's publications have been published in the leading journals and conferences in his field

As preliminary definitions, the h5-index is the h-index for articles published in the last 5 complete years. It is the largest number h such that h articles published in 2018-2023 have at least h citations each. As a concrete example, if a journal has 100 publications published within the period 2018-2023 each having at least 100 citations or more, the journal's h5-index will be 100. The Impact Factor (IF) is a number quantifying the number of citations an article receives in the 2 years since its publication. an IF > 10 indicates that the journal belongs to the top 1.9% journals worldwide and an IF > 6 indicates that the journal belongs to the top 5.41% [Exhibit 40]. Dr. Griffiths's scientific articles have been published in the leading venues in Machine Learning and the Natural Sciences, which include:

- Advances in Neural Information Processing (NeurIPS): h5-index: 309 and the 9th ranked publication venue across all areas of research indexed by Google Scholar (Exhibit 21). Dr. Griffiths has authored two articles in NeurIPS [Exhibit 1, Exhibit 12, Exhibit 13]

- The International Conference on Machine Learning (ICML): A top tier conference in machine learning research with a Google Scholar h5-index of 254 and the 17th ranked publication venue across all fields of research indexed by Google Scholar [Exhibit 21]. Dr. Griffiths authored one article on machine learning in ICML [Exhibit 20].
- The Journal of Artificial Intelligence Research (JAIR): A top journal in machine learning and artificial intelligence with an Impact Factor of 2.776. Dr. Griffiths authored one article on Bayesian optimization in JAIR [Exhibit 1, Exhibit 29].
- The Journal of Machine Learning Research (JMLR): JMLR is the premier journal for machine learning research with a h5-index of 106 and an Impact Factor of 5.177. Dr. Griffiths authored one article on Bayesian optimization in JMLR [Exhibit 1, Exhibit 17].
- Accounts of Chemical Research: A top journal in chemistry [Exhibit 21] with a h5-index of 163, an Impact Factor of 18.3, and the 84th ranked publication venue across all fields of research indexed by Google Scholar [Exhibit 21]. Dr. Griffiths authored one paper on machine learning applications to chemistry in Accounts of Chemical Research [Exhibit 1, Exhibit 14].
- Chemical Science: The flagship journal for the Royal Society of Chemistry with a h5-index of 132 and an Impact Factor of 9.969. Dr. Griffiths has published two papers on machine learning applications in chemistry in Chemical Science [Exhibit 1, Exhibit 11].
- The Astrophysical Journal: A leading journal in astrophysics with a h5-index of 169, an Impact Factor of 5.874, and the 68th ranked publication venue across all fields of research indexed by Google Scholar [Exhibit 21]. Dr. Griffiths has published one paper on applications of Gaussian processes to high-energy astrophysics in the Astrophysical Journal [Exhibit 1, Exhibit 18].
- Machine Learning: Science and Technology (MLST): A journal published by the Institute of Physics with an Impact Factor of 6.8. Dr. Griffiths has published one paper on Bayesian optimization in MLST [Exhibit 1, Exhibit 15].
- Applied AI Letters: A new journal published by Wiley with an Impact Factor of 1.2. Dr. Griffiths has published one paper on machine learning in Applied AI Letters [Exhibit 1, Exhibit 16]
- Electronic Imaging: A leading conference in applications of computer vision. Dr. Griffiths has coauthored 4 papers on applications of AI to the fine arts in Electronic Imaging [Exhibit 1, Exhibit 21, Exhibit 22, Exhibit 23, Exhibit 24].

Prof. XYZ, the examiner of Dr. Griffiths's PhD thesis has verified that Dr. Griffiths's work has been published in leading venues in the field.

"*Dr. Griffiths's first author work was published in prestigious international journals in their respective fields: The Astrophysical Journal (Impact Factor: 5.874), Chemical Science (Impact Factor: 9.969), and Machine Learning: Science and Technology (Impact Factor: 6.013). Dr. Griffiths was also a core contributor to several other papers during his PhD published in venues such as The International Conference on Machine Learning (h5-index: 237) and The Accounts of Chemical Research (Impact Factor: 24.47).* "

(Prof. XYZ, Professor of XYZ, University of XYZ)

2.2.3 Dr. Griffiths's scientific articles have been cited significantly more than the articles of his peers

It is worth noting that in Kazarian v. USCIS, 596 F.3d 1115, 1121 (9th Cir. 2010) the court confirmed that the act of publication was sufficient, and rejected the Service's view that petitioner must show other scholars have cited his work. Based on the aforementioned, the above-stated is sufficient evidence to meet the plain language of the criterion of evidence of authorship of scholarly articles in professional or major trade publications or other major media. However, Dr. Griffiths's work has also been cited extensively as will be described here.

The works authored by Dr. Griffiths have attained significantly more citations than the average for the field as gauged by the impact factor of the journals his work has been published in. Dr. Griffiths's articles in Chemical Science have achieved 200+ citations and 34 citations respectively in the two years since their publication [Exhibit 1], significantly higher than the average of 9.969 for the impact factor. His paper in the Journal of Artificial Intelligence Research has attained 115 citations in under two years since its publication, significantly higher than the impact factor of 2.776. His paper in Accounts of Chemical Research has attained 50+ citations significantly more than the impact factor of 18.3. Dr. Griffiths's paper in JMLR has received 15 citations, which is higher than the Impact Factor of 5.177. Lastly, Dr. Griffiths's papers in MLST and the Astrophysical Journal have received 35 citations, and 17 citations respectively, also higher than the Impact Factors of 6.8 and 5.874. When taking all publications of Dr. Griffiths into account, his 1042 citations gathered so far place him within the top 1% percentile of scholars in Computer Science according to the ESI ranking [Exhibit 39].

2.3 Evidence that Dr. Griffiths has been asked to judge the work of others in machine learning and the natural sciences

Dr. Griffiths has been a reviewer for the top journals and conferences in machine learning and the sciences [Exhibit 35]. Dr. Griffiths has reviewed a total of 49 scientific articles including:

- Advances in Neural Information Processing (NeurIPS): h5-index: 309 and the 9th ranked publication venue across all areas of researched indexed by Google Scholar (Exhibit 21). Dr. Griffiths has reviewed 10 articles for this conference.
- Nature Machine Intelligence: With an Impact Factor of 23.8, Nature Machine Intelligence is a leading journal in machine learning and artificial intelligence. Dr. Griffiths has reviewed 2 articles for this journal.
- Nature Communications Chemistry: With an Impact Factor of 5.9, Nature Communications Chemistry is a leading journal in the natural sciences. Dr. Griffiths has reviewed 1 article for this journal.

- npj Computational Materials: With an Impact Factor of 12.256 it is a leading journal in computational science. Dr. Griffiths has reviewed 1 article for this journal.
- IEEE Transactions on Evolutionary Computation: With an Impact Factor of 16.497, it is a leading journal in optimization algorithms. Dr. Griffiths has reviewed 1 article for this journal.
- IEEE Transactions on Intelligent Systems: With an Impact Factor of 6.94, it is a leading journal in artificial intelligence and expert systems. Dr. Griffiths has reviewed 2 articles for this journal.
- Chemical Science: With a h5-index of 132 and an Impact Factor of 9.969, it is the flagship journal of the Royal Society of Chemistry and a top journal in the field of chemistry. Dr. Griffiths has reviewed 6 articles for this journal.
- Machine Learning: Science and Technology: With an Impact Factor of 6.8, it is a top journal in machine learning applied to the natural sciences. Dr. Griffiths has reviewed 2 articles for this journal.
- Applied Artificial Intelligence: With an Impact Factor of 2.8, it is a widely known journal in applications of artificial intelligence. Dr. Griffiths has reviewed 1 article for this journal.
- Journal of Chemical Information and Modeling: With an Impact Factor of 5.6, it is a well-known journal in applications of computational techniques to chemistry. Dr. Griffiths has reviewed 1 article for this journal.
- RSC Advances: With a h5-index of 109 and an Impact Factor of 4.036, it is a leading journal in chemistry. Dr. Griffiths has reviewed 3 articles for this journal.
- Entropy: With a h5-index of 78 and an Impact Factor of 2.7, it is a prestigious journal in machine learning and physics. Dr. Griffiths has reviewed 1 article for this journal.
- PeerJ Computer Science: With an Impact Factor of 3.8, it is a popular journal in computer science. Dr. Griffiths has reviewed 1 article for this journal.
- Applied Physics Reviews: With a h5-index of 84 and an Impact Factor of 19.527, it is a prestigious journal in physics Dr. Griffiths reviewed 1 article for this journal.
- Journal of Physics: Condensed Matter: With a h5-index of 55 and an Impact Factor of 2.7, it is a top journal in condensed matter physics. Dr. Griffiths has reviewed 1 article for this journal.
- Plasma Physics and Controlled Fusion: With a h5-index of 42 and an Impact factor of 2.2, it is a leading journal in plasma physics. Dr. Griffiths has reviewed 2 articles for this journal.
- Chemical Communications: With a h5-index of 109 and an Impact Factor of 4.9, it is a leading journal in the chemical sciences. Dr. Griffiths has reviewed 4 articles for this journal.
- Journal of Computational Chemistry: With an Impact Factor of 3.0, it is a leading journal in computational chemistry. Dr. Griffiths has reviewed 1 article for this journal.
- Reaction Chemistry and Engineering: With a h5-index of 43 and an Impact Factor of 3.9, it is a leading journal in the chemical sciences. Dr. Griffiths has reviewed 3 articles for this journal.

- Current Opinion in Chemical Engineering: With an Impact Factor of 6.117, it is a prestigious journal in the chemical sciences. Dr. Griffiths has reviewed 1 article for this journal.
- Digital Discovery: It is a new journal on machine learning in the natural sciences. Dr. Griffiths has reviewed 1 article for this journal.
- Environmental Research Communications: With an Impact Factor of 2.9, it is a leading journal in environmental science. Dr. Griffiths has reviewed 1 article for this journal.
- Minerals: With an impact factor of 2.5, it is a leading journal in the earth sciences. Dr. Griffiths has reviewed 1 article for this journal.
- Neuromorphic Computing and Engineering: Is a new journal on neural networks and machine learning. Dr. Griffiths has reviewed 1 article for this journal.

Further details of the journals Dr. Griffiths has reviewed for are provided in [Exhibit 36]. An Impact Factor > 10 indicates that the journal belongs in the top 1.9% of all journals worldwide [Exhibit 40]. In particular, the fact that Dr. Griffiths was sought as a reviewer for Nature Machine Intelligence (IF: 23.8), IEEE Transactions on Evolutionary Computation (IF: 16.497), and npj Computational Materials (IF: 12.256) indicates that Dr. Griffiths's expertise in Machine Learning and the Natural Sciences has been recognized at the highest level. A point that is supported by Dr. XYZ, Prof. XYZ, and Prof. XYZ:

"*Dr. Griffiths has also reviewed for the leading journals and conferences in the field of machine learning and the sciences. As an example in the field of machine learning, from 2021-2023 Dr. Griffiths served as an expert reviewer for Neural Information Processing Systems (NeurIPS), the world's premier machine learning conference, receiving close to 10,000 submissions each year and maintaining an acceptance rate of ca. 20%. Given the highly competitive nature of NeurIPS, articles published in this venue are perceived to be of even higher merit than those published in machine learning journals. In terms of machine learning applications in the sciences, Dr. Griffiths has also reviewed for top journals including Nature Machine Intelligence which maintains very high standards in accepting only the most impactful papers. It should be emphasised that only expert reviewers are recruited for the task of gauging the impact of papers submitted to such journals.*"

(Prof. XYZ, Professor of XYZ, University of XYZ)

"*Dr. Griffiths has served as a reviewer for over 50 scientific articles and has received a trusted reviewer award from the Institute of Physics. Some of the most important journals and conferences Dr. Griffiths has reviewed for have included the Nature Machine Intelligence journal, the Chemical Science journal, and the Neural Information Processing Systems conference, all of which maintain very high standards for reviewer selection.*"

(Prof. XYZ, Professor of XYZ, University of XYZ)

"*In addition to his research contributions, Dr. Griffiths has also reviewed extensively for the leading journals and conferences in the field, a position of great responsibility that helps to maintain the standard and integrity of the peer review process. Dr. Griffiths has reviewed for top journals and conferences including Nature Machine Intelligence, Nature Communications Chemistry, npj Computational Materials, and NeurIPS. I should emphasise that only leading researchers in their field are invited to review for such prestigious venues.*"

(Prof. XYZ, Professor of XYZ, University of XYZ)

Additionally, as an expert in the field of Machine Learning and the Natural Sciences, Dr. Griffiths has acted as a member of the program committee (expert reviewer) for the world's three premier international machine learning conferences: NeurIPS, ICML, and ICLR, where Dr. Griffiths was sought as a disinterested outside party:

- Program Committee (Expert Reviewer) for NeurIPS conference 2021-2022, the world's premier machine learning conference: `https://nips.cc/Conferences/2021/DatasetBenchmarkReviewers` and `https://neurips.cc/Conferences/2022/DatasetBenchmarkProgramCommittee`
- Program Committee member: Machine learning in Healthcare Workshops 2020-2022. Selected to be a reviewer for the Machine Learning for Healthcare Workshop at NeurIPS for 3 years in a row (https://proceedings.mlr.press/v193/parziale22a/parziale22a.pdf)
- Program Committee member: 2021-22 ELLIS Workshop on Machine Learning for Molecules
- Program Committee member: 2022 ICML Workshop on AI4Science
- Program Committee member: 2022 ICLR Workshop on Deep Generative Models for Highly Structured Data
- Program Committee member: 2020 NeurIPS Workshop on Machine Learning for Molecules
- Program Committee member: 2021 NeurIPS workshop on AI4Science
- Program Committee member: 2021 NeurIPS Workshop on Machine Learning and the Physical Sciences
- Program Committee member: 2022 NeurIPS Workshop on Gaussian Processes, Spatiotemporal Modeling, and Decision-making System

Furthermore, Dr. Griffiths was awarded the trusted reviewer status by the Institute of Physics (IOP) in recognition of "an exceptionally high level of peer review competency" [Exhibit 41]. Evidence of Dr. Griffiths's review activity and program committee service is provided in [Exhibit 35].

2.4 Evidence of published material about Dr. Griffiths and his work in Machine Learning and the Natural Sciences in professional or major trade publications or other major media

Dr. Griffiths's work has been featured in professional and major trade publications including Synced and MIT Technology Review as well as on YouTube by Relay Therapeutics, a US-based drug discovery

company. Additionally, Dr. Griffiths's work has been cited by academic publications that themselves had been published in highly prestigious venues underscoring how Dr. Griffiths's work has been leveraged from applications ranging from drug discovery to the ATLAS experiments at CERN.

2.4.1 Dr. Griffiths's work has been featured in Synced

Dr. Griffiths's work on the mathematical capabilities of ChatGPT:

- Frieder S, Pinchetti L, Chevalier A, **Griffiths R.R**, Salvatori T, Lukasiewicz T, Petersen PC, and Berner J. Mathematical capabilities of ChatGPT. *Advances in Neural Information Processing Systems*, 2023.

has been featured in Synced: `https://syncedreview.com/2023/02/03/genius-or-subpar-ai-mathematician-new-studyquestions-chatgpts-mathematical-capabilities/`. Founded in March 2014, Synced is China's first media entity that focuses on reporting machine intelligence and related technologies. Synced is currently the industry's most influential content producer, principled to produce professional, authoritative, and edifying content relating to the fields of Artificial Intelligence, robotics, neuroscience, and other forefront technologies. Synced is dedicated to providing a platform for those who wish to learn more about cutting-edge technology and discover how to deal with the upcoming waves of technological revolution. It is a platform that proactively initiates discussions regarding human-technology relationship that seek to inspire imagination and creativity, meanwhile encouraging readers to reflect upon the interactive future of humanity and technology. On China's largest social network and content sharing platform, WeChat, Synced has more than 190,000 subscribers with more than 50,000 readers per day. Synced also maintains over 20,000 daily total page visit on other platforms such as Baidu, TouTiao.com, Netease, and Sohu. Based on subscriber and third-party feedback, its professionalism, practicality and thoughtfulness are widely recognized and commended by company executives, experts, scholars, well-known investors, and industry practitioners.

Synced is also the key content provider for Tencent, Baidu, and TouTiao.com, winning the title of Huxiu's Top Ten Content Provider of 2015 and TouTiao's Best vertical-Media of 2015. Synced proudly served as APEC Global VR Summit's chief technology media, the one and only Chinese Media partner of AI frontier conference in the silicon valley, and was invited to report in the Brain Forum 2016 in Switzerland as the only Chinese media. Synced has conducted numerous in-depth interviews with industry leaders who provided valuable insight on industry dynamics and expertise. Past interviewees include the godfather of Reinforcement Learning professor Richard Sutton from University of Alberta, Coursera co-founder and professor at Stanford University Andrew Ng, Professor Eric P. Xing from Carnegie Mellon University, Microsoft Research's chief Artificial Intelligence scientist Li Deng, Professor Qiang Yang from Hong Kong University of Science and Technology, the founders of MXNet, Duke University's vice provost for research Lawrence Carin, Professor Jack Gallant from UC Berkeley, and Nobel Laureate Randy Schekman. It has also reported on Baidu, Google, IBM, Microsoft, among other major technology companies, alongside many outstanding Artificial Intelligence companies and robotics startups around the world. Further details are available in [Exhibit 42]

2.4.2 Dr. Griffiths's work has been featured in MIT Technology Review

Dr. Griffiths's work on the recovery of underdrawings and ghost-paintings via style transfer by deep convolutional neural networks:

- Bourached A, Cann G, **Griffiths R.R**, Stork D. Recovery of Underdrawings and Ghost-Paintings via Style Transfer by Deep Convolutional Neural Networks: A Digital Tool for Art Scholars, *Electronic Imaging*, 2021.

has been featured in MIT Technology Review: `https://www.technologyreview.com/2019/09/20/132929/this-picasso-painting-had-neverbeen-seen-before-until-a-neural-network-painted-it/`. Founded at the Massachusetts Institute of Technology in 1899, MIT Technology Review is a world-renowned, independent media company whose insight, analysis, reviews, interviews, and live events explain the newest technologies and their commercial, social, and political impacts. MIT Technology Review derives authority from its relationship to the world's foremost technology institution and from its editors' deep technical knowledge, capacity to see technologies in their broadest context, and unequaled access to leading innovators and researchers. It is a digitally-oriented, independent media company whose readers are curious technology enthusiasts—a global audience of business and thought leaders, innovators and early adopters, entrepreneurs, and investors. Every day, the publication provides an authoritative filter for the flood of information about technology. MIT Technology Review is the first to report on a broad range of new technologies, informing its audiences about how important breakthroughs will impact their careers and their lives. Further details are available in [Exhibit 42].

2.4.3 Dr. Griffiths's work has been featured and used by Relay Therapeutics

Dr. Griffiths's work on FlowMO, a library for Gaussian processes in chemistry:

- **Griffiths R.R**, Moss H. Gaussian Process Molecular Machine Learning with FlowMO. *NeurIPS Workshop on Machine Learning for Molecules*, 2020.

has been featured and used by Relay Therapeutics, a US drug discovery company. A description of the use of FlowMO by Relay Therapeutics may be found at 12:08 in the following video `https://www.youtube.com/watch?v=5PS6I6NjmDk)`. Further details are available in [Exhibit 42].

2.4.4 Dr. Griffiths's work has been cited in professional publications

International researchers have extensively relied on Dr. Griffiths's research and have referenced and cited it in their own works, further substantiating Dr. Griffiths's national and international recognition for his extraordinary ability and significant accomplishments in the field of Machine Learning and the Natural Sciences. The following lists a subset of the most significant of the 101 academic publications that have cited Dr. Griffiths's HEBO algorithm:

- Search for a new Z'gauge boson events with the ATLAS experiment. ATLAS Collaboration, 2023. arXiv preprint arXiv:2301.09342,(https://arxiv.org/abs/2301.09342) - applied the HEBO algorithm.

- Gryffin: An algorithm for Bayesian optimization of categorical variables informed by expert knowledge. Häse, F., Aldeghi, M., Hickman, R.J., Roch, L.M. and Aspuru-Guzik, A., 2021. Applied Physics Reviews, 8(3), p.031406. (Cited by 82, Impact Factor 19.527).

- Reinforced few-shot acquisition function learning for Bayesian optimization. Hsieh, B.J., Hsieh, P.C. and Liu, X., 2021. Advances in Neural Information Processing Systems, 34, pp.7718-7731. (Cited by 7, Conference h5-index: 309 – 9th ranked publication venue on Google Scholar across all disciplines)

- PFNs4BO: in-context learning for Bayesian optimization. Samuel Müller, Matthias Feure, Noah Hollmann, and Frank Hutter. 2023. In Proceedings of the 40th International Conference on Machine Learning (ICML'23), Vol. 202. JMLR.org, Article 1056, 25444–25470. (Conference h5-index: 254 - 17th ranked publication venue on Google Scholar across all disciplines) - directly built on the HEBO algorithm.

The following lists a subset of the most significant of the more than 320 academic publications that have cited Dr. Griffiths's constrained Bayesian optimization paper:

- Bayesian reaction optimization as a tool for chemical synthesis. Shields, B.J., Stevens, J., Li, J., Parasram, M., Damani, F., Alvarado, J.I.M., Janey, J.M., Adams, R.P. and Doyle, A.G., 2021. Nature, 590(7844), pp.89-96. (Cited by 388, Impact Factor: 64.8 - world's leading academic publication venue)

- BoTorch: A framework for efficient Monte-Carlo Bayesian optimization. Balandat, M., Karrer, B., Jiang, D., Daulton, S., Letham, B., Wilson, A.G. and Bakshy, E., 2020. Advances in Neural Information Processing Systems, 33, pp.21524-21538. (Cited by 583, Conference h5-index: 309 – 9th ranked publication venue on Google Scholar across all disciplines)

The following lists a citation from the AstraZeneca AI research group, who used the FlowMO library in their paper on human-in-the-loop de novo molecular design:

- Sundin, I., Voronov, A., Xiao, H., Papadopoulos, K., Bjerrum, E.J., Heinonen, M., Patronov, A., Kaski, S. and Engkvist, O., 2022. Human-in-the-loop assisted de novo molecular design. Journal of Cheminformatics, 14(1), pp.1-16. (Impact Factor: 8.6).

Given that an Impact Factor > 10 indicates a journal is in the top 1.9% of publications [Exhibit 40], Nature, Applied Physics Reviews, and Advances in Neural Information Processing Systems, are unequivocally and widely considered leading, prestigious scientific journals and conference proceedings [Exhibit 38]. Further details on media are available in [Exhibit 42].

3 The final merits of Dr. Griffiths's extraordinary ability

In accordance with the Kazarian opinion, the second step of the two-part approach is a final merits determination that considers all of the evidence in the context of whether or not the petitioner has demonstrated:

- A level of expertise indicating that Dr. Griffiths is "one of that small percentage who have risen to the very top of the field of endeavor." 8 C.F.R. §204.5(h)(2) – section 3.1.
- Dr. Griffiths's sustained national or international acclaim and that his achievements have been recognized in the field of his expertise. 8 C.F.R. §204.5(h)(3) – section 3.2.

3.1 Dr. Griffiths has risen to the very top of the field of machine learning and the natural sciences

By virtue of his research contributions, both academically, and industrially via the the use of his research in the pharmaceutical sector, Dr. Griffiths is recognised by several notable referees as to have risen to the very top of the field of Machine Learning and the Natural Sciences:

"*Given Dr. Griffiths's contributions in machine learning and the natural sciences, I have no hesitation in stating that Dr. Griffiths is among the very top of his research field. Dr. Griffith's contributions have had wide-ranging impact not only in academia as evidenced by his publications and citation count, but also in industry, where his work has been implemented by pharmaceutical companies such as AstraZeneca (Sweden) and Relay Therapeutics (USA).*"

(Prof. XYZ, Professor of XYZ, University of XYZ)

"*In conclusion, Ryan-Rhys Griffiths's research has helped to inform the progression of projects at Lawrence Livermore National Laboratory and his continued work at Meta Research will no doubt continue to benefit our work. Dr. Griffiths has made outstanding contributions of great impact to the field of machine learning and the natural sciences marking him out as having risen to the very top of his field.*"

(Prof. XYZ, Professor of XYZ, University of XYZ)

"*Dr. Griffith's research contributions demonstrate that he has risen to the very top of the field of machine learning and natural sciences. In the past year alone he has had 2 papers accepted to NeurIPS 2023, the world's top tier international machine learning conference.*"

(Prof. XYZ, Professor of XYZ, University of XYZ)

Additionally, the publications authored by Dr. Griffiths have been cited over 1000 times [Exhibit 2], meaning that he occupies a position in the top 1% of researchers in computer science as per the ESI index [Exhibit 39].

3.2 Dr. Griffiths has sustained national and international acclaim in his field of expertise

Dr. Griffiths's research record not only indicates contributions of international acclaim but also that Dr. Griffiths has sustained said contributions. Dr. Griffiths's articles have been cited over 450 times in the

past year alone [Exhibit 2] highlighting an increasing trend in the impact of his research and international recognition amongst the scientific community. Furthermore, Dr. Griffiths's work has recently attained widespread media attention and has seen use in the pharmaceutical sector. Dr. Griffiths's sustained national and international acclaim is supported by his referees:

"*Dr. Griffith's contributions were recently featured in mainstream Chinese media. Taken together, these contributions firmly demonstrate that Dr. Griffiths has had, and I fully expect will continue to have, sustained international acclaim in his field.*"

(Prof. XYZ, Professor of XYZ, University of XYZ)

"*Furthermore, Dr. Griffiths has sustained his contributions to the international research community over time, as evidenced by achieving over 450 citations in the past year alone. It is typically considered an achievement to have a single paper accepted to NeurIPS, but this year Dr. Griffiths had two papers accepted to this top tier conference. I have no hesitation in recommending that Ryan-Rhys Griffiths be awarded an EB-1A green card based on his outstanding research scholarship in machine learning.*"

(Prof. XYZ, Professor of XYZ, University of XYZ)

"*Dr. Griffiths has also garnered 200+ citations in 2022 and 480+ citations in 2023. These achievements together provide grounded evidence of Dr. Griffiths's contributions of international acclaim as well as his ability to sustain them.*"

(Prof. XYZ, Professor of XYZ, University of XYZ)

4 Conclusion

Dr. Griffiths has risen to the very top of of his field as a recognized expert in machine learning and the natural sciences and aims to continue working in the USA in his field of research expertise. As evidenced in supporting letters from notable domain experts, Dr. Griffiths's research on Bayesian optimization will contribute significant benefits to the pharmaceutical and machine learning industries in the USA. In the former case, through the acceleration of drug discovery campaigns and in the latter case through speedups to general machine learning algorithms.

As such, Dr. Griffiths fully satisfies the requirements and regulations listed in INA Section 203(b)(1)(A) and 8 CFR Section 204.5(h) and the reviewer is kindly asked to approve Dr. Griffiths's petition for permanent residence under the category of alien of extraordinary ability.

Please contact me at the following address for any additional evidence.

Sincerely,

NB: Do not forget to sign your name here!

Dr. Ryan-Rhys Griffiths

Address: XX Street, San Francisco, CA XXXXX
Tel: XXXXXXXXX
Email: xxxxxxxxx@gmail.com

Statement from Dr. Griffiths detailing plans on how he intends to continue work in the United States

10 September 2025

I, Ryan-Rhys Griffiths, am the beneficiary of this I-140 Immigrant Petition for Alien Worker, seeking EB1-A classification as an individual of extraordinary ability. I have extensive experience in the field of machine learning and the sciences and I intend to continue my research in this field in the United States.

I plan to continue my role as a research scientist at Meta where my research focusses on the development of novel Bayesian optimization and deep learning methods that will enable machine learning models to be trained faster and in a more cost-effective manner, accelerating the rate at which discoveries in artificial intelligence can be made.

Permanent residence in the United States would grant me increased flexibility to travel to international conferences to disseminate the findings of my open-source research and provide benefit to the broader scientific community without concern for recurring visa stamping.

My area of expertise, machine learning and the sciences, will contribute advances to healthcare and renewable energy technologies, by accelerating the rate at which novel drug compounds and molecular materials are discovered, providing a better quality of life for US citizens and people worldwide. In addition, I hope to provide benefits to the national economy by improving the state-of-the-art in machine learning hyperparameter optimization which would expedite the rate at which machine learning models can be trained providing tangible benefits to US business infrastructure.

I would be very grateful to be granted the chance to contribute my expertise in machine learning and the sciences to benefit the US economy and healthcare system.

Yours Sincerely,

NB: Do not forget to sign your name here!

Ryan-Rhys Griffiths

Address: XX Street, San Francisco, CA XXXXX
Tel: XXXXXXXXX
Email: xxxxx@gmail.com

List of Exhibits

Academic and Professional Background

Exhibit 1: Curriculum Vitae of Dr. Ryan-Rhys Griffiths

Exhibit 2: Google Scholar Profile of Dr. Ryan-Rhys Griffiths

Supporting Letters

Exhibit 3: Supporting letter and bio from Prof XYZ

Exhibit 4: Supporting letter and bio from Prof XYZ

Exhibit 5: Supporting letter and bio from Prof XYZ

Exhibit 6: Supporting letter and bio from Prof XYZ

Exhibit 7: Supporting letter and bio from Dr. XYZ

Exhibit 8: Supporting letter and bio from Prof XYZ

Key scientific Publications Authored by Dr. Griffiths

Exhibit 9: A peer-reviewed publication authored by Dr. Griffiths on generative models of molecules:

- **Griffiths R.R** and Hernández-Lobato J.M., Constrained Bayesian Optimization for Automatic Chemical Design using Variational Autoencoders. *Chemical Science* 11(2), pp.577-586, 2020.

Exhibit 10: A peer-reviewed publication authored by Dr. Griffiths on the Heteroscedastic Evolutionary Bayesian Optimisation (HEBO) algorithm:

- Cowen-Rivers A., Lyu W., Tutunov R., Wang Z., Grosnit A., **Griffiths R.R**, Hao J., Wang J., Bou-Ammar H., HEBO: Pushing The Limits of Sample-Efficient Hyper-parameter Optimisation. *Journal of Artificial Intelligence Research*, 74, pp.1269-1349, 2022.

Exhibit 11: A peer-reviewed publication authored by Dr. Griffiths on the use of multioutput Gaussian processes to discover novel photoswitch molecules:

- **Griffiths R.R**, Greenfield JL, Thawani AR, Jamasb A, Moss HB, Bourached A, Jones P, McCorkindale W, Aldrick AA, Fuchter M, Lee AA., Data-Driven Discovery of Molecular Photoswitches with Multioutput Gaussian Processes. *Chemical Science*, 2022.

Exhibit 12: A peer-reviewed publication by Dr. Griffiths on GAUCHE: A software library for Gaussian processes in Chemistry:

- **Griffiths R.R**, Klarner L, Moss HB, Ravuri A, Truong S, Du Y, Stanton S, Tom G, Rankovic B, Jamasb A, Schwartz J, Deshwal A, Tripp A, Kell G, Frieder S, Bourached A, Chan A, Moss J, Guo C, Durholt JP, Chaurasia S, Park JW, Strieth-Kalthoff F, Lee AA, Cheng B, Aspuru-Guzik, A, Schwaller P, Tang J, GAUCHE: A Library for Gaussian Processes in Chemistry. *NeurIPS*, 2023.

Exhibit 13: A peer-reviewed publication by Dr. Griffiths on the mathematical capabilities of ChatGPT:

- Frieder S, Pinchetti L, Chevalier A, **Griffiths R.R**, Salvatori T, Lukasiewicz T, Petersen PC, and Berner J, 2023. Mathematical capabilities of ChatGPT. *NeurIPS*, 2023.

Exhibit 14: A peer-reviewed publication authored by Dr. Griffiths on the ASAP software library for machine learning on molecules and materials:

- Cheng B, **Griffiths R.R**, Wengert S, Kunkel C, Stenczel T, Zhu B, Deringer VL, Bernstein N, Margraf JT, Reuter K, Csanyi G. Mapping Materials and Molecules. *Accounts of Chemical Research*, 2020.

Exhibit 15: A peer-reviewed publication authored by Dr. Griffiths on Bayesian optimization under heteroscedastic, aleatoric uncertainty:

- **Griffiths R.R**, Aldrick A, Garcia-Ortegon M, Lalchand V, Lee, AA. Achieving Robustness to Aleatoric Uncertainty with Heteroscedastic Bayesian Optimisation. *Machine Learning: Science and Technology*, 2021.

Exhibit 16: A peer-reviewed publication authored by Dr. Griffiths on machine learning models for human motion prediction:

- Bourached A, **Griffiths R.R**, Gray R, Jha A, Nachev P. Generative Model-Enhanced Human Motion Prediction. *Applied AI Letters*, 2021.

Exhibit 17: A peer-reviewed publication authored by Dr. Griffiths on the use of compositional optimizers for Bayesian optimization:

- Grosnit A, Cowen-Rivers A, Tutunov R, **Griffiths R.R**, Wang J, Bou-Ammar H. Are We Forgetting About Compositional Optimisers in Bayesian Optimisation. *Journal of Machine Learning Research*, 2021.

Exhibit 18: A peer-reviewed publication authored by Dr. Griffiths on the use of Gaussian processes for modelling black hole accretion discs:

- **Griffiths R.R**, Jiang J, Buisson D, Wilkins D, Gallo L, Ingram, A, Lee AA, Grupe D, Kara M, Parker ML, Alston W, Bourached A, Cann G, Young A, Komossa S. Modelling the Multiwavelength Variability of Mrk-335 using Gaussian Processes. *The Astrophysical Journal*, 2021.

Exhibit 19: A peer-reviewed publication authored by Dr. Griffiths introducing a theoretical model of nanoparticle self-assembly at electrochemical solid/liquid interfaces:

- Zagar C, **Griffiths R.R**, Podgornik R, Kornyshev AA. On the Voltage-Controlled Self-Assembly of NP Arrays at Electrochemical Solid/Liquid Interfaces. *Journal of Electroanalytical Chemistry*, 2020.

Exhibit 20: A peer-reviewed publication authored by Dr. Griffiths introducing a machine learning algorithm and theoretical analysis of optimal sensor placement:

- Grant J, Boukouvalas A, **Griffiths R.R**, Leslie D, Vaikili S, Munoz de Cote E. Adaptive Sensor Placement for Continuous Spaces. *ICML*, 2019.

Exhibit 21: First page of a peer-reviewed publication authored by Dr. Griffiths on the recovery of lost artworks using machine learning:

- Bourached A, Cann G, **Griffiths R.R**, Stork D. Recovery of Underdrawings and Ghost-Paintings via Style Transfer by Deep Convolutional Neural Networks: A Digital Tool for Art Scholars, *Electronic Imaging*, 2021.

Exhibit 22: A peer-reviewed publication authored by Dr. Griffiths on the use of AI for inferring meaning from artworks:

- Kell G, **Griffiths R.R**, Bourached A, Stork D. Extracting Associations and Meanings of Objects Depicted in Artworks through Bi-Modal Deep Networks, *Electronic Imaging*, 2022.

Exhibit 23: A peer-reviewed publication authored by Dr. Griffiths using computer vision to identify subjects in artworks:

- Stork D, Bourached A, Cann G, **Griffiths R.R**, Computational Identification of Significant Actors in Paintings through Symbols and Attributes, *Electronic Imaging*, 2021.

Exhibit 24: A peer-reviewed publication authored by Dr. Griffiths on recovering lost artwork through machine learning and computer vision:

- Cann G, Bourached A, **Griffiths R.R**, Stork D. Resolution Enhancement in the Recovery of Underdrawings Via Style Transfer by Generative Adversarial Deep Neural Networks, *Electronic Imaging*. 2021.

Exhibit 25: Dr. Griffiths's PhD thesis on applications of Gaussian processes and machine learning in the natural sciences:

- **Griffiths R.R**, Applications of Gaussian Processes at Extreme Lengthscales: From Molecules to Black Holes. PhD Thesis, *University of Cambridge*, 2022.

Exhibit 26: A publication authored by Dr. Griffiths on high-dimensional Bayesian optimization using variational autoencoders

- **Griffiths R.R**, Grosnit A, Tutunov R, Maraval AM, Cowen-Rivers A, Yang L, Lin Z, Lyu W, Chen Z, Wang J, Peters J, Bou-Ammar H. High-Dimensional Bayesian Optimisation with Variational Autoencoders and Deep Metric Learning. *arXiv*, 2021.

Exhibit 27: A publication authored by Dr. Griffiths on machine learning for human motion prediction:

- Bourached A, Gray R, **Griffiths R.R**, Jha A, Nachev P. Hierarchical Graph-Convolutional Variational AutoEncoding for Generative Modelling of Human Motion. *arXiv*, 2021.

Exhibit 28: A publication authored by Dr. Griffiths on the use of Bayesian optimization for enhancing the yields of chemical reactions:

- Ranković, B, **Griffiths, R.R**, Moss, HB and Schwaller, P. Bayesian optimisation for additive screening and yield improvements in chemical reactions–beyond one-hot encodings. *arXiv*, 2022.

Exhibit 29: A peer-reviewed publication authored by Dr. Griffiths on inferring missing links in supply chain networks using graph-based machine learning:

- Aziz A, Kosasih EE, **Griffiths R.R**, Brintrup A. Data Considerations in Graph Representation Learning for Supply Chain Networks. *ICML Workshop on Machine Learning for Data: Automated Creation, Privacy, Bias*, 2021

Exhibit 30: A peer-reviewed publication authored by Dr. Griffiths on high dimensional Bayesian optimization considering invariant transformations:

- Verma E, Chakraborty S, **Griffiths R.R**. *ICML Workshop on Adaptive Experimental Design and Active Learning in the Real World*, 2022.

Exhibit 31: A peer-reviewed publication authored by Dr. Griffiths on FlowMO, a software library for Gaussian processes in machine learning:

- **Griffiths R.R**, Moss H. Gaussian Process Molecular Machine Learning with FlowMO. *NeurIPS Workshop on Machine Learning for Molecules*, 2020.

Exhibit 32: A publication authored by Dr. Griffiths on dataset bias when applying machine learning in the natural sciences:

- **Griffiths R.R**, Schwaller P, Lee AA. Dataset Bias in the Natural Sciences: A Case Study in Chemical Reaction Prediction and Synthesis Design. *NeurIPS Workshop on Critiquing and Correcting Trends in Machine Learning*, 2018.

Exhibit 33: Dr. Griffiths's master's thesis on a theoretical model of a nanoplasmonic electrovariable mirror system:

- **Griffiths R.R**. A Theory of a Self-Assembling Electrovariable Smart Mirror. MSci Thesis, *Imperial College London*, 2016.

Other

Exhibit 34: Proof of acceptance of Dr. Griffiths's 2023 NeurIPS papers.

Exhibit 35: Proof of 49 scientific reviews undertaken by Dr. Griffiths in 23 conferences and journals on Machine Learning and the Natural Sciences.

Exhibit 36: Further details of the journals Dr. Griffiths has conducted reviews for.

Exhibit 37: Most popular articles in physical and theoretical chemistry published in Chemical Science in 2022.

Exhibit 38: Number of citations of the top articles in the top 100 publications worldwide

Exhibit 39: Number of citations of top 1% authors percentile according to the ESI index.

Exhibit 40: Journal Impact Factor ranking percentiles.

Exhibit 41: Trusted reviewer certificate issued to Dr. Griffiths by the Institute of Physics.

Exhibit 42: Media articles covering Dr. Griffiths's work.

Exhibit 43: Confirmation of PhD degree and MPhil degree of Dr. Griffiths issued by the University of Cambridge, alongside confirmation of MSci degree and transcript of Dr. Griffiths issued by Imperial College London.

Exhibit 44: Offer letter of Dr. Griffiths as a researcher at Meta Platforms, Inc.

Exhibit 1

Curriculum Vitae of Dr. Ryan-Rhys Griffiths

Ryan-Rhys Griffiths

Phone: 6463303983 (M)
Email: ryangriff123@gmail.com
LinkedIn: https://www.linkedin.com/in/ryan-rhys-griffiths-689b73128/
Twitter: https://twitter.com/ryan_rhys
GitHub: https://github.com/Ryan-Rhys

Employment

Meta Research, Menlo Park, CA, USA Aug 2022 - Present

Postdoctoral Research Scientist

- Organization: Central Applied Science
- Director: Dr. Eytan Bakshy
- Specialism: Bayesian Optimization, Gaussian Processes
- 2 Papers Accepted to NeurIPS 2023
- Area Chair for NeurIPS AI4Science Workshop
- Google Scholar citations: 1042
- Google Scholar h-index: 14
- Google Scholar i10-index: 16
- Awarded an O-1 visa

Huawei Noah's Ark Lab, London, UK Oct 2020 - Oct 2021

AI Research Scientist

- Department: AI Theory Group
- Director: Prof. Haitham Bou-Ammar
- Specialism: Optimization, Bayesian Deep Learning, Antibody Design, Biological Sequence Design,
- 1st Place in the 2020 NeurIPS Black-Box Optimization Competition
- Papers published in JMLR and JAIR

Secondmind Labs, Cambridge, UK Oct 2017 - Oct 2018

Machine Learning Engineer

- Department: Multiagent Systems Group
- Manager: Dr. Alexis Boukouvalas
- Specialism: Bayesian Nonparametrics and Reinforcement Learning
- Paper published at ICML 2019

Education

University of Cambridge Oct 2018 - Aug 2022

PhD, Machine Learning and Physics

- PhD Thesis: *Applications of Gaussian Processes at Extreme Lengthscales: From Molecules to Black Holes*
- Department: Physics, Theory of Condensed Matter, Cavendish Laboratory
- Supervisor: Dr. Alpha Lee
- Specialism: Astronomical time series, Gaussian processes, ML4Science
- Papers published in the Astrophysical Journal, Chemical Science, Accounts of Chemical Research and Machine Learning: Science and Technology
- Featured a 1-year break to work full-time as a Research Scientist at Huawei Noah's Ark Lab

University of Cambridge Oct 2016 - Oct 2017

MPhil, Machine Learning and Machine Intelligence

- MPhil Thesis: Constrained Bayesian Optimization for Automatic Chemical Design
- Department: Engineering, Machine Learning Group
- Supervisor: Prof. José Miguel Hernández-Lobato
- Paper published in Chemical Science
- Coursework: Distinction grades in Probabilistic Machine Learning, Reinforcement Learning, Statistical Spoken Dialogue Systems, Speech Recognition and Natural Language Processing
- 1st Place in Kaggle Classification Competition

Imperial College London Oct 2012 - Jun 2016

MSci, Chemistry, 1st Class

- MSci Thesis: A Theory of a Self-Assembling Electrovariable Smart Mirror
- Department: Chemistry, Theoretical Chemical Physics Group
- Supervisor: Prof. Alexei Kornyshev
- Paper published in the Journal of Electroanalytical Chemistry
- Constructed a mathematical model of a nanophotonic, electrochemical mirror-window system for novel sensing applications in renewable energy, trace analyte detection and counter-terrorism
- Extended Thomas-Fermi theory to account for the effect of finite penetration of a point charge into the body of a material
- Coursework: Organic, Inorganic and Physical Chemistry, ranked in the top 10 students in finals

Coursera/EdX

- 32 certifications with topics including Linear Algebra, Bayesian Methods for Machine Learning, Deep Learning, Statistical Learning, Algorithms and Data Structures, Computational Neuroscience and Natural Language Processing

Other Positions

Mila - Quebec AI Institute, Montreal, Canada Jan 2022 - Jun 2022

Visiting Machine Learning Researcher

- Supervisor: Prof. Jian Tang
- Specialism: Molecular Machine Learning, Sequence Design
- Recipient of a $25,000 Samsung AI fellowship

Oxia Palus, London, UK Oct 2019 - Present

Machine Learning Research Associate

- Oxia Palus is an AI art collective using machine learning to recover lost artwork
- Research has been featured in MIT Technology Review

University College London, UK Jun 2015 - Oct 2015

Machine Learning Research Student

- Department: CSML, Gatsby Unit
- Supervisors: Prof. John Shawe-Taylor and Dr. Guy Lever
- Supervised Learning on the Alzheimer's Disease Neuroimaging Initiative (ADNI) biomedical dataset

Imperial College London, UK Jun 2014 - Oct 2014

Theoretical Condensed Matter Physics Research Student

- Department: Chemistry, Theoretical Chemical Physics Group
- Supervisor: Prof. Alexei Kornyshev
- Built a mathematical model of an electroactuator system for use in voltage-controlled micro and nano-robotics
- Placement funded through an EPSRC vacation bursary award

Consulting Experience

Independent, London, UK Oct 2017 - Aug 2022

Machine Learning

- Designed and delivered a course on Probabilistic Machine Learning for G-Research
- Delivered a course on Python and Machine Learning for the Schmidt Data Science Residency Programme at Cambridge University.
- Designed and delivered a Deep Learning seminar series for JPMorgan.
- Designed and delivered a Data Science course for Morgan Stanley.
- Lead Instructor for the Deep Learning course at the STFC Data Intensive, Artificial Intelligence and Machine Learning Summer School.

Teaching Assistant, University of Cambridge, UK Oct 2018 - Mar 2019

- Demonstrator for the Natural Sciences Tripos course on Scientific Computing

Publications

Refereed Journal Papers

[J1] Grosnit A, Cowen-Rivers A, Tutunov R, **Griffiths RR**, Wang J, Bou-Ammar H. Are We Forgetting About Compositional Optimisers in Bayesian Optimisation. *Journal of Machine Learning Research*, 2021.

[J2] Cowen-Rivers A, Lyu W, Tutunov R, Wang Z, Grosnit A, **Griffiths RR**, Hao J, Wang J, Bou-Ammar H. HEBO: Pushing The Limits of Sample-Efficient Hyperparameter Optimisation. *Journal of Artificial Intelligence Research*, 2022.

[J3] Bourached A, **Griffiths RR**, Gray R, Jha A, Nachev P. Generative Model-Enhanced Human Motion Prediction. *Applied AI Letters*, 2021.

[J4] **Griffiths RR**, Aldrick A, Garcia-Ortegon M, Lalchand V, Lee, AA. Achieving Robustness to Aleatoric Uncertainty with Heteroscedastic Bayesian Optimisation. *Machine Learning: Science and Technology*, 2021.

[J5] **Griffiths RR**, Jiang J, Buisson D, Wilkins D, Gallo L, Ingram, A, Lee AA, Grupe D, Kara M, Parker ML, Alston W, Bourached A, Cann G, Young A, Komossa S. Modelling the Multiwavelength Variability of Mrk-335 using Gaussian Processes. *The Astrophysical Journal*, 2021.

[J6] **Griffiths RR**, Hernández-Lobato JM. Constrained Bayesian Optimization for Automatic Chemical Design using Variational Autoencoders. *Chemical Science*, 2020.

[J7] Zagar C, **Griffiths RR**, Podgornik R, Kornyshev AA. On the Voltage-Controlled Self-Assembly of NP Arrays at Electrochemical Solid/Liquid Interfaces. *Journal of Electroanalytical Chemistry*, 2020.

[J8] Cheng B, **Griffiths RR**, Wengert S, Kunkel C, Stenczel T, Zhu B, Deringer VL, Bernstein N, Margraf JT, Reuter K, Csanyi G. Mapping Materials and Molecules. *Accounts of Chemical Research*, 2020.

[J9] **Griffiths RR**, Greenfield JL, Thawani AR, Jamasb A, Moss HB, Bourached A, Jones P, McCorkindale W, Aldrick AA, Fuchter M, Lee AA. Data-Driven Discovery of Molecular Photoswitches with Multioutput Gaussian Processes. *Chemical Science*, 2022.

[J10] Ranković, B, **Griffiths, RR**, Moss, HB and Schwaller, P. Bayesian optimisation for additive screening and yield improvements–beyond one-hot encoding. *Digital Discovery*, 2023.

Refereed Conference Papers

[C1] **Griffiths RR**, Klarner L, Moss HB, Ravuri A, Truong S, Du Y, Stanton S, Tom G, Rankovic B, Jamasb A, Schwartz J, Deshwal A, Tripp A, Kell G, Frieder S, Bourached A, Chan A, Moss J, Guo C, Durholt JP, Chaurasia S, Park JW, Strieth-Kalthoff F, Lee AA, Cheng B, Aspuru-Guzik, A, Schwaller P, Tang J, GAUCHE: A Library for Gaussian Processes in Chemistry. *NeurIPS*, 2023 (Main Track - 26.1% Acceptance Rate).

[C2] Frieder S, Pinchetti L, Chevalier A, **Griffiths RR**, Salvatori T, Lukasiewicz T, Petersen PC, and Berner J, 2023. Mathematical capabilities of ChatGPT. *NeurIPS*, 2023. (Datasets and Benchmarks Track 2023 - 32.7% Acceptance Rate).

[C3] Grant J, Boukouvalas A, **Griffiths RR**, Leslie D, Vaikili S, Munoz de Cote E. Adaptive Sensor Placement for Continuous Spaces. *ICML*, 2019 (22.6% Acceptance Rate).

[C4] Kell G, **Griffiths RR**, Bourached A, Stork D. Extracting Associations and Meanings of Objects Depicted in Artworks through Bi-Modal Deep Networks, *Electronic Imaging*, 2022.

[C5] Stork D, Bourached A, Cann G, **Griffiths RR**, Computational Identification of Significant Actors in Paintings through Symbols and Attributes, *Electronic Imaging*, 2021.

[C6] Cann G, Bourached A, **Griffiths RR**, Stork D. Resolution Enhancement in the Recovery of Underdrawings Via Style Transfer by Generative Adversarial Deep Neural Networks, *Electronic Imaging*. 2021.

[C7] Bourached A, Cann G, **Griffiths RR**, Stork D. Recovery of Underdrawings and Ghost-Paintings via Style Transfer by Deep Convolutional Neural Networks: A Digital Tool for Art Scholars, *Electronic Imaging*, 2021.

[C8] Bourached A, Cann G, **Griffiths RR**, Eriksson J, Stork D., Style Transfer for Improved Visualization of Underdrawings and Ghost Paintings: An Application to a Work by Vincent van Gogh, *Electronic Imaging*, 2023.

Refereed Workshop Papers

[W1] Verma E, Chakraborty S, **Griffiths RR**. High-Dimensional Bayesian Optimization with Invariance. *ICML Workshop on Adaptive Experimental Design and Active Learning in the Real World*, 2022.

[W2] Aziz A, Kosasih EE, **Griffiths RR**, Brintrup A. Data Considerations in Graph Representation Learning for Supply Chain Networks. *ICML Workshop on Machine Learning for Data: Automated Creation, Privacy, Bias*, 2021

[W3] **Griffiths RR***, Moss H*. Gaussian Process Molecular Machine Learning with FlowMO. *NeurIPS Workshop on Machine Learning for Molecules*, 2020 (Contributed Talk - top 5%, * joint first authorship).

[W4] Bourached A, **Griffiths RR**, Gray R, Jha A, Nachev P. Generative Model-Enhanced Human Motion Prediction. *NeurIPS Workshop on Interpretable Inductive Biases and Physically-Structured Learning*, 2020.

[W5] **Griffiths RR**, Jones P, McCorkindale W, Aldrick AA, Jamasb A, Day B. Benchmarking Scalable Active Learning Strategies on Molecules. *ICLR Workshop on Fundamental Science in the Era of AI* 2020.

[W6] **Griffiths RR**, Thawani AR, Elijosius R. Enhancing the Diversity of Molecular Machine Learning Benchmarks: An Open-Source Dataset for Molecular Photoswitches. *ICLR Workshop on Fundamental Science in the Era of AI*, 2020.

[W7] **Griffiths RR**, Schwaller P, Lee AA. Dataset Bias in the Natural Sciences: A Case Study in Chemical Reaction Prediction and Synthesis Design. *NeurIPS Workshop on Critiquing and Correcting Trends in Machine Learning*, 2018.

[W8] **Griffiths RR**, Hernández-Lobato JM. Constrained Bayesian Optimization for Automatic Chemical Design. *NIPS Workshop on Bayesian Optimization for Science and Engineering*, 2017.

Technical Reports

[R1] **Griffiths RR**. A Theory of a Self-Assembling Electrovariable Smart Mirror. *arXiv*, 2017.

Preprints

[P1] **Griffiths RR***, Grosnit A*, Tutunov R*, Maraval AM*, Cowen-Rivers A, Yang L, Lin Z, Lyu W, Chen Z, Wang J, Peters J, Bou-Ammar H. High-Dimensional Bayesian Optimisation with Variational Autoencoders and Deep Metric Learning. *arXiv*, 2021. (* joint first authorship)

[P2] Bourached A, Gray R, **Griffiths RR**, Jha A, Nachev P. Hierarchical Graph-Convolutional Variational AutoEncoding for Generative Modelling of Human Motion. *arXiv*, 2021.

PhD Thesis

[T1] **Griffiths RR**, Applications of Gaussian Processes at Extreme Lengthscales: From Molecules to Black Holes. PhD Thesis, *University of Cambridge*, 2022.

Reviewing

• NeurIPS	2021, 2022, 2023
• AISTATS	2024
• Nature Machine Intelligence	2020, 2023
• Nature Communications Chemistry	2022
• npj Computational Materials	2022
• AutoML Conference	2023
• IEEE Intelligent Systems	2021
• IEEE Transactions on Evolutionary Computation	2020
• Entropy	2022
• PeerJ Computer Science	2022
• Neuromorphic Computing and Engineering	2022
• Applied Artificial Intelligence	2022
• Applied Physics Reviews	2021
• Classical and Quantum Gravity	2023

- Journal of Physics: Condensed Matter 2021
- Plasma Physics and Controlled Fusion 2021, 2022
- Machine Learning: Science and Technology 2021
- Chemical Science 2019, 2020, 2021, 2022, 2023
- Chemical Communications 2020, 2021, 2022
- RSC Advances 2020, 2021, 2022
- Journal of Computational Chemistry 2022
- Reaction Chemistry and Engineering 2021, 2022
- Current Opinion in Chemical Engineering 2022
- Digital Discovery 2022
- Environmental Research and Communications 2021
- Minerals 2022

Program Committee

- Area Chair for NeurIPS Workshop on AI4Science 2023
- NeurIPS Workshop on Gaussian Processes 2022
- NeurIPS Workshop on AI4Science 2021, 2022
- ICLR Workshop on Deep Generative Models 2022
- NeurIPS Workshop on Machine Learning for Molecules 2020
- NeurIPS Workshop on Machine Learning for Healthcare 2020, 2021, 2022
- NeurIPS Workshop on Machine Learning and the Physical Sciences 2021

Invited Talks

- *Bayesian Optimization over Generative Models of Materials and Molecules*, Meta AI Research, San Francisco, USA, 2023
- *Applications of Gaussian Processes at Extreme Lengthscales: From Molecules to Black Holes*, Tecnológico de Monterrey, Monterrey, Mexico, 2023
- *GAUCHE: A Library for Gaussian Processes in Chemistry*, Evonik Industries AG, Essen, Germany, 2022
- *Applications of Gaussian Processes at Extreme Lengthscales: From Molecules to Black Holes*, EPFL, Lausanne, Switzerland, 2022
- *Modelling the Multiwavelength Variability of Markarian 335 using Gaussian Processes*, Institute of Astronomy, Cambridge, UK, 2020
- *Automatic Chemical Design*, Wolfson Research Event, Cambridge, UK, 2019
- *The Rise of Machine Learning and its Relevance for the Natural Sciences*, Good-enough College, London, UK, 2019
- *Constrained Bayesian Optimization for Automatic Chemical Design*, NIPS Workshop on Bayesian Optimization for Science and Engineering, Long Beach, USA, 2017

Technical Skills

- **Programming Languages**: Python, MATLAB/Octave
- **Technologies/Frameworks**: PyTorch, TensorFlow, Theano, GPflow, BoTorch, GPyTorch, Azure
- **Operating System Tools**: UNIX shell, bash scripting

Awards

- MILA-Samsung Scholarship: $25,000 — Jan 2022
- Huawei Noah's Ark Lab Prize - Best PhD research scientist — Feb 2021
- G-Research Prize - Best draft PhD thesis: £5,000 — Mar 2020
- NeurIPS 2019 Travel Grant — Dec 2019
- EPSRC Vacation Bursary Award: £2,200 — Jul 2014

References

- **Prof. Alán Aspuru-Guzik**, Director, Acceleration Consortium, Professor of Computer Science, Professor of Chemical Engineering and Applied Chemistry, University of Toronto
  Email: aspuru@utoronto.ca
- **Prof. Sergei Kalinin**, Weston Fulton Professor of Materials Science and Engineering, Blavatnik Award Laureate, Physics, 2018, Feynman Prize, 2022, Foreign member, Academia Europaea, Fellow MRS, MSA, IoP, APS, IEEE, AVS, Foresight Institute
  Email: sergei2@utk.edu Phone Number: +1 (865) 207 7885
- **Prof. David Ginsbourger**, Director of Studies in Statistics, Co-director of the Institute of Mathematical Statistics and Actuarial Sciences, University of Bern
  Email: ginsbourger@stat.unibe.ch Phone Number: (+41) 31 684 88 42
- **Prof. Bingqing Cheng**, Assistant Professor, IST Austria
  Email: bingqing.cheng@ist.ac.at
- **Prof. Philippe Schwaller**, Assistant Professor of Digital Chemistry, EPFL
  Email: philippe.schwaller@epfl.ch Phone Number: (+41) 21 693 20 56

Interests and Achievements

Chess

- FIDE Master with 2 International Master Norms
- Former British Junior Champion (U18)
- Five-time Irish Junior Champion (U14, U16, U19)
- Board 3 for the Irish Men's Team at the 2012 Chess Olympiad in Istanbul
- Board 1 for Cambridge in the 2017 Varsity Match

Other

- Captain of the Wolfson College University Challenge (televised quiz show) Team for the 2019-20 season: Episode Link
- Long-distance running: RunBritain handicap of 2.2
- Latin Dance: Cuban Salsa, Bachata, Cross-Body Salsa.

Exhibit 2

Google Scholar Profile of Dr. Ryan-Rhys Griffiths

Ryan-Rhys Griffiths

Meta Research
Machine Learning
Physics
Chemistry
Bayesian Optimization
AI for Science

	All	Since 2018
Citations	1042	1039
h-index	14	14
i10-index	16	16

0 articles 6 articles

not available available

Based on funding mandates

TITLE	CITED BY	YEAR
Constrained Bayesian Optimization for Automatic Chemical Design using Variational Autoencoders RR Griffiths, JM Hernández-Lobato Chemical Science 11 (2), 577-586	334 *	2020
Mathematical Capabilities of ChatGPT S Frieder, L Pinchetti, RR Griffiths, T Salvatori, T Lukasiewicz, ... NeurIPS 2023	194 *	2023
HEBO: Pushing the Limits of Sample-Efficient Hyper-Parameter Optimisation AI Cowen-Rivers, W Lyu, R Tutunov, Z Wang, A Grosnit, RR Griffiths, ... Journal of Artificial Intelligence Research 74, 1269-1349	115 *	2022
Mapping Materials and Molecules B Cheng, RR Griffiths, S Wengert, C Kunkel, T Stenczel, B Zhu, ... Accounts of Chemical Research 53 (9), 1981-1991	87	2020
High-Dimensional Bayesian Optimisation with Variational Autoencoders and Deep Metric Learning RR Griffiths*, A Grosnit*, R Tutunov*, AM Maraval*, AI Cowen-Rivers, ... arXiv preprint arXiv:2106.03609	48 *	2021
Achieving Robustness to Aleatoric Uncertainty with Heteroscedastic Bayesian Optimisation RR Griffiths, AA Aldrick, M Garcia-Ortegon, V Lalchand Machine Learning: Science and Technology 3 (1), 015004	35 *	2021
Data-Driven Discovery of Molecular Photoswitches with Multioutput Gaussian Processes RR Griffiths, JL Greenfield, AR Thawani, AR Jamasb, HB Moss, ... Chemical Science 13, 13541 - 13551	34 *	2022
Gaussian Process Molecule Property Prediction with FlowMO HB Moss*, RR Griffiths* NeurIPS 2020: Workshop on ML4Molecules	26 *	2020
GAUCHE: A Library for Gaussian Processes in Chemistry RR Griffiths, L Klarner, HB Moss, A Ravuri, S Truong, B Rankovic, Y Du, ... NeurIPS 2023	21 *	2022
Dataset Bias in the Natural Sciences: A Case Study in Chemical Reaction Prediction and Synthesis Design RR Griffiths, P Schwaller, AA Lee arXiv preprint arXiv:2105.02637	19 *	2021

TITLE	CITED BY	YEAR
Adaptive Sensor Placement for Continuous Spaces JA Grant, A Boukouvalas, RR Griffiths, DS Leslie, S Vakili, EM De Cote ICML 2019	18	2019
Modeling the Multiwavelength Variability of Mrk 335 Using Gaussian Processes RR Griffiths, J Jiang, DJK Buisson, D Wilkins, LC Gallo, A Ingram, ... The Astrophysical Journal 914 (2), 144	17	2021
Generative Model-Enhanced Human Motion Prediction A Bourached, RR Griffiths, R Gray, A Jha, P Nachev Applied AI Letters 3 (2), e63	16	2022
Are We Forgetting about Compositional Optimisers in Bayesian Optimisation? A Grosnit, AI Cowen-Rivers, R Tutunov, RR Griffiths, J Wang, ... Journal of Machine Learning Research, 22(160), 1-78.	15	2021
Recovery of Underdrawings and Ghost-Paintings via Style Transfer by Deep Convolutional Neural Networks: A Digital Tool for Art Scholars A Bourached, G Cann, RR Griffiths, DG Stork Electronic Imaging 2021	13 *	2021
Data Considerations in Graph Representation Learning for Supply Chain Networks A Aziz, EE Kosasih, RR Griffiths, A Brintrup ICML 2021: Workshop on ML4Data	10	2021
Computational Identification of Significant Actors in Paintings through Symbols and Attributes DG Stork, A Bourached, GH Cann, RR Griffiths Electronic Imaging 2021	8	2021
High-Dimensional Bayesian Optimization with Invariance E Verma, S Chakraborty, RR Griffiths	7 *	2000
Bayesian Optimisation for Additive Screening and Yield Improvements-Beyond One-Hot Encoding B Ranković, RR Griffiths, H Moss, P Schwaller Digital Discovery	6 *	2023
Extracting Associations and Meanings of Objects Depicted in Artworks through Bi-Modal Deep Networks K Gregory, G Ryan-Rhys, B Anthony Electronic Imaging 34, 1-14	5 *	2022

Exhibit 3

Supporting letter and bio from Prof. XYZ

Exhibit 4

Supporting letter and bio from Prof. XYZ

Exhibit 5

Supporting letter and bio from Prof. XYZ

Exhibit 6

Supporting letter and bio from Prof. XYZ

Exhibit 7

Supporting letter and bio from Prof. XYZ

Exhibit 8

Supporting letter and bio from Prof. XYZ

Exhibit 9

A peer-reviewed publication authored by Dr. Griffiths on generative models of molecules

- **Griffiths R.R** and Hernández-Lobato J.M., Constrained Bayesian Optimization for Automatic Chemical Design using Variational Autoencoders. *Chemical Science* 11(2), pp.577-586, 2020.

Exhibit 10

A peer-reviewed publication authored by Dr. Griffiths on the Heteroscedastic Evolutionary Bayesian Optimisation (HEBO) algorithm

- Cowen-Rivers A., Lyu W., Tutunov R., Wang Z., Grosnit A., **Griffiths R.R**, Hao J., Wang J., Bou-Ammar H., HEBO: Pushing The Limits of Sample-Efficient Hyper-parameter Optimisation. *Journal of Artificial Intelligence Research*, 74, pp.1269-1349, 2022.

Exhibit 11

A peer-reviewed publication authored by Dr. Griffiths on the use of multioutput Gaussian processes to discover novel photoswitch molecules.

- **Griffiths R.R**, Greenfield JL, Thawani AR, Jamasb A, Moss HB, Bourached A, Jones P, McCorkindale W, Aldrick AA, Fuchter M, Lee AA., Data-Driven Discovery of Molecular Photoswitches with Multioutput Gaussian Processes. *Chemical Science*, 2022.

Exhibit 12

A peer-reviewed publication by Dr. Griffiths on GAUCHE: A software library for Gaussian processes in Chemistry

- **Griffiths R.R**, Klarner L, Moss HB, Ravuri A, Truong S, Du Y, Stanton S, Tom G, Rankovic B, Jamasb A, Schwartz J, Deshwal A, Tripp A, Kell G, Frieder S, Bourached A, Chan A, Moss J, Guo C, Durholt JP, Chaurasia S, Park JW, Strieth-Kalthoff F, Lee AA, Cheng B, Aspuru-Guzik, A, Schwaller P, Tang J, GAUCHE: A Library for Gaussian Processes in Chemistry. *NeurIPS*, 2023.

Exhibit 13

A peer-reviewed publication by Dr. Griffiths on the mathematical capabilities of ChatGPT

- Frieder S, Pinchetti L, Chevalier A, **Griffiths R.R**, Salvatori T, Lukasiewicz T, Petersen PC, and Berner J, 2023. Mathematical capabilities of ChatGPT. *NeurIPS*, 2023.

Exhibit 14

A peer-reviewed publication authored by Dr. Griffiths on the ASAP software library for machine learning on molecules and materials

- Cheng B, **Griffiths R.R**, Wengert S, Kunkel C, Stenczel T, Zhu B, Deringer VL, Bernstein N, Margraf JT, Reuter K, Csanyi G. Mapping Materials and Molecules. *Accounts of Chemical Research*, 2020.

Exhibit 15

A peer-reviewed publication authored by Dr. Griffiths on Bayesian optimization under heteroscedastic, aleatoric uncertainty

- **Griffiths R.R**, Aldrick A, Garcia-Ortegon M, Lalchand V, Lee, AA. Achieving Robustness to Aleatoric Uncertainty with Heteroscedastic Bayesian Optimisation. *Machine Learning: Science and Technology*, 2021.

Exhibit 16

A peer-reviewed publication authored by Dr. Griffiths on machine learning models for human motion prediction

- Bourached A, **Griffiths R.R**, Gray R, Jha A, Nachev P. Generative Model-Enhanced Human Motion Prediction. *Applied AI Letters*, 2021.

Exhibit 17

A peer-reviewed publication authored by Dr. Griffiths on the use of compositional optimizers for Bayesian optimization

- Grosnit A, Cowen-Rivers A, Tutunov R, **Griffiths R.R**, Wang J, Bou-Ammar H. Are We Forgetting About Compositional Optimisers in Bayesian Optimisation. *Journal of Machine Learning Research*, 2021.

Exhibit 18

A peer-reviewed publication authored by Dr. Griffiths on the use of Gaussian processes for modelling black hole accretion discs

- **Griffiths R.R**, Jiang J, Buisson D, Wilkins D, Gallo L, Ingram, A, Lee AA, Grupe D, Kara M, Parker ML, Alston W, Bourached A, Cann G, Young A, Komossa S. Modelling the Multiwavelength Variability of Mrk-335 using Gaussian Processes. *The Astrophysical Journal*, 2021.

Exhibit 19

A peer-reviewed publication authored by Dr. Griffiths introducing a theoretical model of nanoparticle self-assembly at electrochemical solid/liquid interfaces

- Zagar C, **Griffiths R.R**, Podgornik R, Kornyshev AA. On the Voltage-Controlled Self-Assembly of NP Arrays at Electrochemical Solid/Liquid Interfaces. *Journal of Electroanalytical Chemistry*, 2020.

Exhibit 20

A peer-reviewed publication authored by Dr. Griffiths introducing a machine learning algorithm and theoretical analysis of optimal sensor placement

- Grant J, Boukouvalas A, **Griffiths R.R**, Leslie D, Vaikili S, Munoz de Cote E. Adaptive Sensor Placement for Continuous Spaces. *ICML*, 2019.

Exhibit 21

First page of a peer-reviewed publication authored by Dr. Griffiths on the recovery of lost artworks using machine learning

- Bourached A, Cann G, **Griffiths R.R**, Stork D. Recovery of Underdrawings and Ghost-Paintings via Style Transfer by Deep Convolutional Neural Networks: A Digital Tool for Art Scholars, *Electronic Imaging*, 2021.

Exhibit 22

A peer-reviewed publication authored by Dr. Griffiths on the use of AI for inferring meaning from artworks

- Kell G, **Griffiths R.R**, Bourached A, Stork D. Extracting Associations and Meanings of Objects Depicted in Artworks through Bi-Modal Deep Networks, *Electronic Imaging*, 2022.

Exhibit 23

A peer-reviewed publication authored by Dr. Griffiths using computer vision to identify subjects in artworks.

- Stork D, Bourached A, Cann G, **Griffiths R.R**, Computational Identification of Significant Actors in Paintings through Symbols and Attributes, *Electronic Imaging*, 2021.

Exhibit 24

First page of a peer-reviewed publication authored by Dr. Griffiths on recovering lost artwork through machine learning and computer vision

- Cann G, Bourached A, **Griffiths R.R**, Stork D. Resolution Enhancement in the Recovery of Underdrawings Via Style Transfer by Generative Adversarial Deep Neural Networks, *Electronic Imaging*. 2021.

Exhibit 25

Dr. Griffiths's PhD thesis on applications of Gaussian processes and machine learning in the natural sciences

- **Griffiths R.R**, Applications of Gaussian Processes at Extreme Lengthscales: From Molecules to Black Holes. PhD Thesis, *University of Cambridge*, 2022.

Exhibit 26

A publication authored by Dr. Griffiths on high-dimensional Bayesian optimization using variational autoencoders

- **Griffiths R.R**, Grosnit A, Tutunov R, Maraval AM, Cowen-Rivers A, Yang L, Lin Z, Lyu W, Chen Z, Wang J, Peters J, Bou-Ammar H. High-Dimensional Bayesian Optimisation with Variational Autoencoders and Deep Metric Learning. *arXiv*, 2021.

Exhibit 27

A publication authored by Dr. Griffiths on machine learning for human motion prediction

- Bourached A, Gray R, **Griffiths R.R**, Jha A, Nachev P. Hierarchical Graph-Convolutional Variational AutoEncoding for Generative Modelling of Human Motion. *arXiv*, 2021.

Exhibit 28

A publication authored by Dr. Griffiths on the use of Bayesian optimization for enhancing the yields of chemical reactions

- Ranković, B, **Griffiths, R.R**, Moss, HB and Schwaller, P. Bayesian optimisation for additive screening and yield improvements in chemical reactions–beyond one-hot encodings. *arXiv*, 2022.

Exhibit 29

A peer-reviewed publication authored by Dr. Griffiths on inferring missing links in supply chain networks using graph-based machine learning

- Aziz A, Kosasih EE, **Griffiths R.R**, Brintrup A. Data Considerations in Graph Representation Learning for Supply Chain Networks. *ICML Workshop on Machine Learning for Data: Automated Creation, Privacy, Bias*, 2021

Exhibit 30

A peer-reviewed publication authored by Dr. Griffiths on high dimensional Bayesian optimization considering invariant transformations.

- Verma E, Chakraborty S, **Griffiths R.R**. *ICML Workshop on Adaptive Experimental Design and Active Learning in the Real World*, 2022.

Exhibit 31

A peer-reviewed publication authored by Dr. Griffiths on FlowMO, a software library for Gaussian processes in machine learning

- **Griffiths R.R**, Moss H. Gaussian Process Molecular Machine Learning with FlowMO. *NeurIPS Workshop on Machine Learning for Molecules*, 2020.

Exhibit 32

A peer-reviewed publication authored by Dr. Griffiths on dataset bias when applying machine learning in the natural sciences

- **Griffiths R.R**, Schwaller P, Lee AA. Dataset Bias in the Natural Sciences: A Case Study in Chemical Reaction Prediction and Synthesis Design. *NeurIPS Workshop on Critiquing and Correcting Trends in Machine Learning*, 2018.

Exhibit 33

Dr. Griffiths's master's thesis on a theoretical model of a nanoplasmonic electrovariable mirror system

- **Griffiths RR**. A Theory of a Self-Assembling Electrovariable Smart Mirror. *MSci Thesis, Imperial College London*, 2016.

Exhibit 34

Proof of acceptance of Dr. Griffiths's recent NeurIPS papers

Exhibit 35

Proof of 49 scientific reviews undertaken by Dr. Griffiths in 23 conferences and journals on Machine Learning and the Natural Sciences.

Exhibit 36

Details of the journals Dr. Griffiths has reviewed for

Exhibit 37

Most popular 2022 physical and theoretical chemistry articles

Exhibit 38

Number of citations of the top articles in the top 100 publications worldwide

Exhibit 39

Number of citations of top 1% authors percentile according to the ESI index, by research field.

- For Computer Science, having 320 citations as an author classifies one within top 1% of researchers worldwide.

Exhibit 40

Journal Impact Factor Percentiles

Exhibit 41

Institute of Physics Trusted Reviewer Award

Exhibit 42

Media articles covering Dr. Griffiths's work.

Exhibit 43

PhD degree certificate and MPhil degree transcript of Dr. Griffiths issued by the University of Cambridge, alongside confirmation of MSci degree and transcript of Dr. Griffiths issued by Imperial College London.

Exhibit 44

Offer letter of Dr. Griffiths as a researcher at Meta Platforms, Inc.