U.S. Department of Homeland Security
U.S. Citizenship and Immigration Services
2.27.2023

RE: Dr. Ryan-Rhys Griffiths

To Whom it May Concern:

I am pleased to attest to Dr. Ryan-Rhys Griffiths's remarkable research contributions in the field of Machine Learning and the Natural Sciences, specifically in the subfields of Bayesian optimization and Gaussian processes. Dr. Ryan-Rhys Griffiths's original contributions have powerfully impacted the field of Machine Learning and have accelerated the industrial adoption of Bayesian optimization methodologies for scientific applications. His research has attained international acclaim throughout the Machine Learning community and among industry leaders.

As for my own qualifications to provide this recommendation, since 2018 I have served as a Canada 150 Research Chair and full professor of Computer Science, Chemistry, Chemical Engineering, and Materials Science at the University of xxxxx. Prior to this, I was a full professor at xxxxx University from 2013-2018. I received my Ph.D. in Physical Chemistry from University of xxxxx in 2004 under the supervision of William A. Lester Jr. Amongst other recognitions, I received the Google Focused Award for Quantum Computing, the DARPA Young Faculty Award, the Sloan Research Fellowship, The Camille and Henry Dreyfus Teacher-Scholar award, and was selected as one of the best innovators under the age of 35 by the MIT Technology Review. I am a member of the American Physical Society and an elected member of the American Association for the Advancement of Science (AAAS) and received the Early Career Award in Theoretical Chemistry from the American Chemical Society. To date I have authored over 400 journal and conference papers in premier machine learning venues such as NeurIPS as well as premier scientific journals such as Nature and Science. As an expert in the field of machine learning and its applications to the sciences, I am happy to serve as Editor-in-Chief of the journal Digital Discovery and on the editorial board of the journal Machine Learning: Science and Technology.

While serving as a graduate student and subsequently as a Ph.D. researcher at the Univer-

sity of Cambridge from 2016 to 2022, Dr. Griffiths performed critical research in developing Gaussian process and Bayesian optimization methodologies for accelerated materials design and drug discovery. I gained familiarity with Dr. Griffiths's work when serving as editor of the journal Chemical Science where Griffiths's paper on 'Constrained Bayesian Optimization for Automatic Chemical Design using Variational Autoencoders' was accepted in 2019. Griffiths's work built on research introduced by myself and coworkers at the Harvard Intelligent Probabilistic Systems Group in 2016 entitled 'Automatic Chemical Design using a Data-Driven Continuous Representation of Molecules'. I subsequently collaborated with Dr. Griffiths in 2022/23 on the paper 'GAUCHE: A library for Gaussian Processes in Chemistry'. The common theme behind all of these works is to leverage a machine learning methodology known as Bayesian optimization to accelerate materials discovery and drug design. Bayesian optimization may be best described as a tool that attempts to solve expensive optimization problems in a cost-effective manner. Examples of such optimization problems include drug discovery, which may require years of time-intensive wet lab experiments to identify promising drug candidates. Bayesian optimization seeks to accelerate such discovery efforts by making use of a probabilistic machine learning model known as a Gaussian process. To date, successful applications of Bayesian optimization have included machine learning hyperparameter optimization in the field of artificial intelligence, where for example it has accelerated the training time for Google Deepmind's AlphaGo, chemical reaction optimization, where it is used to maximize the yield of chemical reactions, as well as for drug and materials discovery.

Following his Ph.D. work, Dr. Griffiths won a Samsung fellowship as a visiting researcher working with Prof. Jian Tang, a world leader in machine learning applied to drug discovery, at the Montreal institute for Learning Algorithms (MILA). Dr. Griffiths is also currently employed in the Adaptive Experimentation team at Meta, a world leader in the development of Bayesian optimization machinery through the open-source BoTorch library. As a research scientist in this team, Dr. Griffiths continues to improve the infrastructure of BoTorch, the world's leading software library for Bayesian optimization.

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. Additionally, with his paper, "Achieving Robustness to Aleatoric Uncertainty with Heteroscedastic Bayesian Optimization" Dr. Griffiths has advanced Bayesian optimization methodologies that cater for optimization problems with heteroscedastic noise, a core consideration in the search for novel and performant materials that are robust to large-scale manufacturing processes. Specifically, Griffiths introduces a novel acquisition function, aleatoric noise-penalized expected improvement which improves upon incumbent schemes in identifying candidate solutions with low intrinsic measurement error. Most recently, Dr. Griffiths has introduced an open-source software library that

extends the Gaussian process framework to operate on molecular representations and chemical reactions, thus facilitating Bayesian optimization in these settings. The core technical contribution in this work was to introduce Gaussian process kernels that are designed for discrete molecular representations as opposed to the continuous representations commonly encountered in Bayesian optimization problems.

Dr. Griffiths's contributions are particularly relevant for industrial applications. Extending the Gaussian process framework to operate on molecules and chemical reactions opens up the possibility of using Bayesian optimization methodologies to search for novel drug candidates and molecular materials, while his work on high-dimensional Bayesian optimization over structured input spaces allows Bayesian optimization methodologies to be applied to search for objects with non-continuous representations such as novel microchip architectures and optical materials. Dr. Griffiths's Gaussian process software library FlowMO has already received documented use in the chemicals industry by companies such as AstraZeneca and Relay Therapeutics.

Based on Dr. Griffiths's stellar publication record conducting original research in Bayesian optimization as well as the industrial adoption of software he has created, I offer my strongest support of his designation as outstanding research scholar.

Yours Truly,

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Professor, xxxxx
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