

UNIVERSITY OF CALIFORNIA
PRESIDENT'S POSTDOCTORAL FELLOWSHIP PROGRAM
2019-2020

APPLICATION FOR RENEWAL

RETURN BY January 11, 2019

Applicant Name: Ryan J McCarty

State your reason for seeking renewal of your President's Postdoctoral Fellowship:

A second year of fellowship would provide time to ultimately produce a more competitive faculty application. An additional year would allow me to make more progress towards my primary research goal of predicting paramagnetic NMR properties using DFT, resulting in more publications on this work, more chances to establish a reputation from this work, and more time to solve and implement corrections to the many sources of inaccuracy (which prevent widespread use of this approach) that my current work has identified. The diversity outreach component of my fellowship would also benefit, a following year would include more time to widely share the materials I developed this year with professors who teach introductory chemistry courses at community colleges. Lastly an additional year would provide more time to network with current faculty at UC, establishing additional collaborations or advocates for me as a faculty colleague.

Include an updated curriculum vitae

An updated CV is attached separately. A sampling of recent UC assistant professor hires in my research fields indicates that the primary statistically relevant issue with my CV is in number of publications. I need approximately 9 additional publications to be highly competitive for a faculty job offer.

A progress report on your current research and a description of future activities and projected results.

My primary research uses a computational chemistry technique, Density Functional Theory, to predict the nuclear magnetic properties of solid materials, allowing a straightforward approach to interpreting experimental Nuclear Magnetic Resonance results. The eventual goal is to improve the calculations enough so that **paramagnetic** materials can be accurately predicted and the approach broadly used. Significant progress has been made the back-end of the computations: selecting, installing, and learning how to use new software packages; identifying and cataloging experimental data to replicate; writing software scripts to produce calculations across a variety of variables. On the front-end, work is in progress calculating and characterizing the accuracy of the diamagnetic materials which parallel the paramagnetic materials, and recently paramagnetic shift tensors from these same materials have been successfully calculated. Future work includes: a) writing software to generate the NMR ppm shifts from the recently calculated hyperfine coupling tensors and g-tensors. b) Calculating and characterizing the accuracy of a large variety of shifts to identify which factors in a calculation have the largest influence on paramagnetic shifts. c) Incorporate density-corrected DFT or apply other corrections to the predicted

values. d) Write up publications on the calculations performed and the success of the corrections I have implemented.

Anticipated publications:

- 1) Paramagnetic NMR predictions in simple systems using pseudopotentials and GIPAW (with mentor Kieron Burke). Note: This is likely to be several publications on this topic.
- 2) Accuracy of predicted diamagnetic NMR parameters using pseudopotential based GIPAW calculations and diamagnetic NMR parameters (with mentor Kieron Burke)
- 3) Predicting diamagnetic NMR parameters oxide solid state of trace element substitutions using DFT (with collaborators Jingda Zhang, Kieron Burke)

Secondary Research Projects: I have also been working on two additional project which loosely support my primary research and have high potential for additional publications.

- 4) Using the Percus–Yevick approximation to determine the exchange and correlation for an individual electron within a homogenous electron gas (with collaborators Dennis Perchack, Kieron Burke)
- 5) Merging NMR component analysis with known components and machine learning (A recently-started collaboration with three UCI computer science undergraduates and their research mentor Domingos Begalli.)

The outreach project involves creating teaching materials that busy professors can easily add into their introductory chemistry classes so that the students are exposed to the aspects of chemistry which include computers and programming. Thus far I have (nearly) completed a series of lecture slides including developing numerous copyright-free graphics to engage the students, and have an offline version of the website which will serve as the distribution platform. Several undergraduate volunteers have helped test and provide feedback on Excel-based exercises that will be available for professors to incorporate as in class activities or homework. Future work includes getting the website completely online (expected by early March at www.dft123.com), incorporating some additional feedback into the exercises, and compiling the lecture slides into easily downloadable packets for professors. The work has been going faster than expected and so I am planning on using the extra time to test run the lecture slides in community college introductory chemistry classrooms, and possibly add interviews with underrepresented minorities who are also computational chemists onto the website as inspiring role models for students interested in computational chemistry.

Additionally, confirm that you have completed all mandatory trainings.

I completed all mandatory trainings required for my role on the following dates:

UC Ethical Values and Conduct: Completed 7/25/2018

UC Sexual Violence and Sexual Harassment Prevention Training for Staff: Completed 7/30/2018

UC Cyber Security Awareness Training 7/30/2018

UC Cyber Security Awareness Training - Refresher 7/30/2018

Indicate whether you will continue at your present campus location and with your current mentor.

I will continue with my current mentor, Kieron Burke, at my present campus.

In addition to your research plan, please provide the specific steps you are taking to obtain a faculty appointment following this fellowship.

- 1) Networking with UC faculty at multiple institutions.
- 2) I submitted applications for the following UC tenure track positions:
 - a. UCLA Faculty Position, Materials Science and Engineering (Jan 1)
 - b. UCR Assistant Professor, New Chemistries and Materials for Sustainability (Nov 12)
 - c. UCLA Faculty Position, Chemical and Biomolecular Engineering (Nov 1)
 - d. UCI Assistant Professor - Open Faculty Search, Chemistry Department (Oct 15)
 - e. UCSD Assistant Professor, Synthesis, Materials and Chemical Biology (Oct 1)
- 3) Networking with colleagues in my discipline.
 - a. I was elected to, and joined a committee in a national organization (American Ceramics Society: Diversity and Inclusion committee).
 - b. I have made an effort to communicate with professors and researchers at other US universities, at national labs, and at research institutes overseas.
- 4) Met with an associate dean of UCI's engineering school to understand the hiring process and to strategize when would be best to submit my materials for consideration at UC Irvine.

The criteria for renewal are

- 1) **demonstrated progress in research productivity:** See above research progress report.
- 2) **participation in PFPF program activities:** I have participated in all the PFPF program activities that I have been invited to: 2018 Southern California Luncheon (2018-08-28), 2018 Fall Meeting (2018-09-21), and I will be attending the Southern California PFPF winter writing retreat (2019-01-25).
- 3) **availability to be on the job market for UC faculty positions after your training:** I have every plan to be on the job market for UC faculty positions after my postdoctoral training, unless of course I've already got one before then!
- 4) **and the overall expected length of your postdoctoral training:** I expect to be a postdoc for a total of 2-3 years, as is typical for new faculty hires in my field. I anticipate having a competitive faculty application for the Fall 2019 application season, and will pursue external funding opportunities for a third year if I have not secured a faculty position by then.

Signature: 

Date 2019-01-01

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PROGRESS REPORT

RETURN by January 11, 2019

Applicant Name: Ryan J McCarty

Mentor Name/Title: Kieron Burke, Chancellor's Professor

The above-named Fellow is applying for a second year of support from the President's Postdoctoral Fellowship Program.

In your opinion, is this renewal justified?

Yes. Because:

- 1) He has been making a great effort to complete everything described within his original ambitious proposal. However, additional research time is needed to make significant progress on his project.
- 2) Very focused on getting a faculty position at a UC.
- 3) Dedicated to making real change in diversity.
- 4) Renewal would make him competitive for faculty positions.

Provide a brief progress report and evaluation of the Fellow's current research, and state your reasons for supporting this application for renewal.

Research is going very well. We are collecting data, collecting codes, compiling codes, and now running codes. We are on the verge of really exploring the heart of the issue, of why DFT is not working well for NMR spectra of some of these materials. It is likely to take 6 months more to complete this and write it up for a high-impact journal.

Indicate whether or not you will continue to serve as mentor during the second year.

Yes, I will continue to serve as his mentor during the second year.

Evaluate the applicant's prospects for job placement, particularly at the University of California, and how he/she will be affected by renewal.

Ryan's research (setting up software, writing code, compiling datasets, determining the best parameters for calculations) takes a long time to get up and running. An additional year will give him a strong advantage, as with the more time intensive work finished it should be straightforward to produce several journal articles from this work, which is key for job placements. Without renewal, it would be very unlikely that enough research would be accomplished and submitted for Ryan to be competitive on the job market.

Describe your specific plans in the coming year to create or enhance the Fellow's opportunities to obtain a faculty position.

In the current year I have:

- 1) Supported his research by weekly meetings to provide scientific problem solving and discussion, connecting him with undergraduate research assistants to support his research, teaching him DFT through my course.
- 2) Involved Ryan in an additional project that will result in more publications.
- 3) Introduced Ryan to several faculty colleagues at UCs who may become collaborators, and/or and now more likely to support his faculty applications should an opportunity arise.
- 4) Set up a meeting with Ryan and an Associate Dean of Engineering to strategize his internal application to UCI departments, such as materials.
- 5) Introduced Ryan to several non-UC colleagues who are leaders in our field, although they won't influence a faculty position offer, they will likely be valuable to success as a faculty member.

In the coming year I intended to continue the efforts listed above, as well as:

- 1) Try to get Ryan's research accepted in a high-impact journal.
- 2) Continue to network within the UC system to find the right niche for Ryan's background and skill set.
- 3) Try to have Ryan invited to conferences and to give seminars at universities, especially UC's, once sufficient progress has been made on research.

 Chemistry UC Irvine 2019-01-07
Signature Department Campus Date