Jarrod McClean

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Education

2015 **Doctor of Philosophy in Chemical Physics**, *Harvard University*.
Advisor: Alán Aspuru-Guzik

2015 **Master of Arts in Physics**, *Harvard University*.

2015 **Secondary Field in Computational Science and Engineering**, *Harvard University School of Engineering and Applied Sciences*.

2010 **Bachelor of Science in Chemistry**, *University of California, Berkeley*.
GPA 4.0, with Highest Honors and Departmental Citation

Awards/Honors

2015 **Luis W. Alvarez Postdoctoral Fellowship in Computing Sciences**.

2012 **Harvard University Certificate of Distinction in Teaching**.

2011 **Department of Energy Computational Graduate Science Fellowship**.

2011 **NSF Graduate Research Fellowship**, *(Declined)*.

2011 **Robert Karplus Prize in Chemical Physics**.

2010 **UC Berkeley College of Chemistry Departmental Citation**.

2009 **Jean Dreyfus Boissevain Undergraduate Scholarship for Excellence in Chemistry**.

2008 **William A. Giauque Award**.

2007 **Department of Chemistry Bruce Howard Memorial Scholarship**.

Publications and Preprints (Chronological)

[1] P. J. J. O'Malley, R. Babbush, I. D. Kivlichan, J. Romero, **J. R. McClean**, R. Barends, J. Kelly, P. Roushan, A. Tranter, N. Ding, B. Campbell, Y. Chen, Z. Chen, B. Chiaro, A. Dunsworth, A. G. Fowler, E. Jeffrey, E. Lucero, A. Megrant, J. Y. Mutus, M. Neeley, C. Neill, C. Quintana, D. Sank, A. Vainsencher, J. Wenner, T. C. White, P. V. Coveney, P. J. Love, H. Neven, A. Aspuru-Guzik, and J. M. Martinis. Scalable quantum simulation of molecular energies. *Physical Review X*, 6:031007, 2016.

[2] **J. R. McClean**, M. E. Schwartz, J. Carter, and W. A. de Jong. Hybrid quantum-classical hierarchy for mitigation of decoherence and determination of excited states. *arXiv:1603.05681*, 2016.

[3] **J. R. McClean**, J. Romero, R. Babbush, and A. Aspuru-Guzik. The theory of variational hybrid quantum-classical algorithms *New Journal of Physics*, 18(2):023023, 2016.

[4] N. P. Sawaya, M. Smelyanskiy, **J. R. McClean**, and A. Aspuru-Guzik. Error sensitivity to environmental noise in quantum circuits for chemical state preparation. *Journal of Chemical Theory and Computation*, 12(7):3097–3108, 2016.

[5] R. Santagati, J. Wang, S. Paesani, A. A. Gentile, N. Wiebe, **J. R. McClean**, S. Morley-

Short, P. J. Shadbolt, D. Bonneau, J. Silverstone, D. P. Tew, X. Zhou, J. L. O. Brien, and M. G. Thompson. Quantum simulation of hamiltonian spectra on a silicon chip. *(Submitted - Under Review - Science)*, 2016.

[6] R. Babbush, **J. R. McClean**, D. Wecker, A. Aspuru-Guzik, and N. Wiebe. Chemical basis of Trotter-Suzuki errors in quantum chemistry simulation. *Physical Review A*, 91:022311, 2015.

[7] J. Huh, G. G. Guerreschi, B. Peropadre, **J. R. McClean**, and A. Aspuru-Guzik. Boson sampling for molecular vibronic spectra. *Nature Photonics*, (9):615–620, 2015.

[8] **J. R. McClean** and A. Aspuru-Guzik. Clock quantum Monte Carlo technique: An imaginary-time method for real-time quantum dynamics. *Physical Review A*, 91:012311, 2015.

[9] **J. R. McClean** and A. Aspuru-Guzik. Compact wavefunctions from compressed imaginary time evolution. *RSC Advances*, 5(124):102277–102283, 2015.

[10] A. Tranter, S. Sofia, J. Seeley, M. Kaicher, **J.R. McClean**, R. Babbush, P. V. Coveney, F. Mintert, F. Wilhelm, and P. J. Love. The Bravyi-Kitaev transformation: Properties and applications. *International Journal of Quantum Chemistry*, 115(19):1431–1441, 2015.

[11] A. Peruzzo†, **J. R. McClean**†, P. Shadbolt, M.-H. Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik, and J. L. O'Brien. A variational eigenvalue solver on a photonic quantum processor. *Nature Communications*, 5(4213):1–7, 2014.
† - Equal Contribution by Authors

[12] **J. R. McClean**, R. Babbush, P. J. Love, and A. Aspuru-Guzik. Exploiting locality in quantum computation for quantum chemistry. *The Journal of Physical Chemistry Letters*, 5(24):4368–4380, 2014.

[13] M.-H. Yung, J. Casanova, A. Mezzacapo, **J. R. McClean**, L. Lamata, A. Aspuru-Guzik, and E. Solano. From transistor to trapped-ion computers for quantum chemistry. *Scientific Reports*, 4(3589):1–7, 2014.

[14] **J. R. McClean**, J. A. Parkhill, and A. Aspuru-Guzik. Feynman's clock, a new variational principle, and parallel-in-time quantum dynamics. *Proceedings of the National Academy of Sciences*, 110(41):E3901–E3909, 2013.

[15] **J. R. McClean**, C. Stull, C. Farrar, and D. Mascareñas. A preliminary cyber-physical security assessment of the Robot Operating System (ROS). In *SPIE Defense, Security, and Sensing*, pages 874110–874110. International Society for Optics and Photonics, 2013.

[16] D. Y. Zubarev, X. You, **J.R. McClean**, W. A. Lester Jr, and M. Frenklach. Patterns of local aromaticity in graphene oxyradicals. *Journal of Materials Chemistry*, 21(10):3404–3409, 2011.

[17] J. Wang, D. Domin, B. Austin, D. Y. Zubarev, **J. R. McClean**, M. Frenklach, T. Cui, and W. A. Lester Jr. A diffusion Monte Carlo study of the OH bond dissociation of phenol. *The Journal of Physical Chemistry A*, 114(36):9832–9835, 2010.

[18] D. Y. Zubarev, N. Robertson, D. Domin, **J. R. McClean**, J. Wang, W. A. Lester Jr, R. Whitesides, X. You, and M. Frenklach. Local electronic structure and stability

of pentacene oxyradicals. *The Journal of Physical Chemistry C*, 114(12):5429–5437, 2009.

Research Experience

2015- **Luis W. Alvarez Postdoctoral Fellow in Computing Sciences**, *Lawrence Berkeley National Laboratory*, Computational Research Division.
Exploring the applications of quantum computers and information sparse algorithms to quantum chemistry and materials problems.

2010-2015 **Department of Energy Computational Science Graduate Fellow**, *Harvard University*, Advisor: Alán Aspuru-Guzik.
Studying the intersection between quantum information and quantum chemistry by developing new algorithms for both traditional and quantum computation for chemistry.

2008-2010 **Undergraduate Researcher**, *University of California, Berkeley*, Advisor: William A. Lester Jr.
Using *ab initio* methods and density functional theory to characterize the stability of oxyradical species with applications in soot oxidation and mitigation of pollutants in combustion.

2008 **Research Experience for Undergraduates(REU) Researcher**, *Georgia Institute of Technology*, Advisor: C. David Sherrill.
Working on the development of an improved quantum mechanical polarizable forcefield for modeling non-covalent aromatic interactions such as those in drug intercalation or fundamental pi-stacking.

2007 **Undergraduate Researcher**, *University of California, Berkeley*, Advisor: Marcin Majda.
Applying *ab initio* calculations to study bonding between the interfacial layer of water and an electrochemical probe, TEMPO.

Teaching Experience

Fall 2011 **Teaching Fellow for Chemistry 160 - Physical Chemistry**, *Harvard University*, with Prof. Eric Heller.
Awarded Harvard University Certificate of Distinction in Teaching

Spring 2011 **Teaching Fellow for Physical Sciences 1 - Introduction to the Physical Sciences**, *Harvard University*, with Prof. Adam Cohen and Prof. Hongkun Park.

Invited Talks

Aug 2, 2016 **Hybrid quantum-classical computation for chemistry and materials**, *Quantum Lunch Seminar - Los Alamos National Laboratory*.

Jul 13, 2016 **Hybrid quantum-classical computation for chemistry and materials**, *NASA Quantum Artificial Intelligence Group Meeting*.

Jun 22, 2016 **Using quantum computers for materials discovery and energy applications**, *Organization Omitted - Technology Focus Day*.

Jun 13, 2016 **Hybrid quantum-classical computation for chemistry and materials**, *Oak Ridge National Laboratory*.

Mar 2, 2016 **Hybrid Quantum-Classical Algorithms for Large Eigenvalue Problems**, *UC Berkeley Applied Mathematics Seminar*.

Nov 17, 2015 **Beyond Exascale: Quantum Processing Units**, *Supercomputing - DOE National Laboratories Exhibition*.

Sep 16, 2015 **Hybrid Quantum-Classical Algorithms for Solving Problems**, *Intel Parallel Computing Group Meeting.*

Apr 3, 2015 **Using quantum computers to change the way we study chemical problems**, *Computational Research in Boston and Beyond Seminar - MIT.*

Mar 4, 2015 **Variational Quantum Eigensolver: How to Use Any Quantum Device in Your Lab to Perform Quantum Simulation**, *APS March Meeting - Quantum Algorithms.*

Feb 26, 2015 **Variational Quantum Eigensolver: How to use any quantum device in your lab to perform quantum simulation**, *Bilbao Conference on Quantum Simulations - Benasque, Spain.*

Nov 5 2014 **Leveraging technology from quantum computing to better understand classical simulation**, *University of Bristol Physics and Chemistry Colloquium.*

Nov 28 2013 **A variational eigenvalue solver on a quantum processor**, *Heilbronn Quantum Algorithms Meeting – Isaac Newton Institute – University of Cambridge.*
Video Available Online: http://www.newton.ac.uk/seminar/20131128100011001

Nov 12, 2012 **The Blurring Interface Between Quantum Computing and Quantum Chemistry**, *Quantum Computation for Quantum Chemistry: Status, Challenges, and Prospects - Session 2 - Microsoft Research.*
Video Available Online: http://research.microsoft.com/apps/video/default.aspx?id=177461

Contributed Talks

Mar 14, 2016 **Hybrid Quantum-Classical Approach to Molecular Excited States**, *APS March Meeting - Quantum Simulation.*

Mar 4, 2015 **Compact wavefunctions from compressed imaginary time evolution**, *APS March Meeting - Electronic Structure Methods.*

Oct 9, 2013 **Feynman's Clock and taking advantage of quantum computers before they are built**, *Student presentation at ITAMP Joint Quantum Sciences Seminar.*

Sept 8, 2013 **A variational eigenvalue solver on a quantum processor**, *The 22nd International Conference on Parallel Architectures and Compilation Techniques - Quantum Computing Workshop.*

Apr 8 2013 **A variational algorithm on a quantum processor for quantum chemistry**, *Quantum Information Seminar – University of Bristol.*

Sept 9, 2012 **Solving eigenvalue problems with the quantum computer in your lab instead of the quantum computer in your dreams**, *Student presentation at ITAMP Joint Quantum Sciences Seminar.*

Posters

Jul 15, 2014 **Consequences of Orthogonality in Quantum Simulations**, *Department of Energy Computational Graduate Science Fellowship Annual Program Review.*

Jul 25, 2013 **Feynman's Clock, a New Variational Principle, and Parallel-in-Time Quantum Dynamics**, *Department of Energy Computational Graduate Science Fellowship Annual Program Review.*

Aug 2008 **Current Methods for Non-Additive Argon Interactions**, *NSF REU Program Poster Session, Georagia Institute of Technology, Atlanta, GA.*

Jul 26, 2012 **A New Perspective on Quantum Dynamics**, *Department of Energy Computational Graduate Science Fellowship Annual Program Review.*

Mar 24, 2010 **Lithium adsorption on graphene: A diffusion Monte Carlo study**, *Division of Physical Chemistry Poster Session - 2010 American Chemical Society conference in San Francisco, California.*

Mar 23, 2010 **Improvement of the quantum mechanical polarizable force field: Generalization of the exchange term and application to the lattice energy of crystalline benzene**, *Division of Computers in Chemistry Poster Session - 2010 American Chemical Society conference in San Francisco, California.*

Sept 24, 2009 **Pentacene Oxyradical Stability**, *International Conference for Advanced Materials Division BB Poster Session - Rio de Janeiro, Brazil.*

Technical Skills

Programming.
C, C++, Python, Matlab, MPI, OpenMP, CUDA

Data Analysis.
Excel, SQL, Pandas, Matplotlib, scikit-learn, scipy, numpy

Communication.
Experienced presenter with commendations in teaching complex material to students

Mathematical.
Non-linear optimization, statistics, linear algebra, numerical analysis of algorithms, high-dimensional data representation and compression

Citizenship

United States Citizen.