

About Alán

Professor of Chemistry and Computer Science, University of Toronto



Starting July 1st, 2018

Department of Chemistry
Department of Computer Science
University of Toronto

Faculty Member, Vector Institute for Artificial Intelligence
CIFAR Senior Fellow Biologically-Inspired Solar Energy
Program

Canada 150 Research Chair in Theoretical Chemistry (2018-)
Professor, University of Toronto (2018-)

Chief Scientific Officer, Zapata Computing
Chief Vision Officer, Kebotix
Scientific Advisor, Kyulux

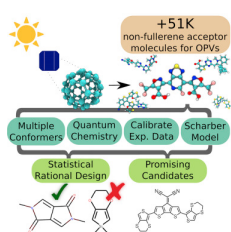
Professor, Harvard University (2013-2018)
Associate Professor, Harvard University (2010-2013)
Assistant Professor, Harvard University (2006-2010)
Postdoctoral Researcher, UC Berkeley (2005-2006)
Ph.D., UC Berkeley (2004)
B.Sc., Universidad Nacional Autónoma de México (1999)

Major Honors and Awards

2018	Google Focused Award for Quantum Computing
2018	Canada 150 Research Chair in Theoretical and Quantum Chemistry
2017	Elected Fellow of the American Association for the Advancement of Science (AAAS)
2017-2018	Invited Member of the World Economic Forum's Global Future Council on Advanced Materials
2016	Per-Olov Löwdin Lecturer, Uppsala University
2015	Canadian Institute for Advanced Research (CIFAR) Senior Fellow
2015	Korea Advanced Institute of Technology EEWS Distinguished Lecturer
2015	Vannevar Bush Faculty Fellowship , (Formerly National Security Science and Engineering Faculty Fellowship)
2015	Member of Origins of Life Initiative, Harvard University
2015	Information Science and Technology Center Distinguished Lecturer, Colorado State University
2015	Associate Editor, Chemical Science
2015	Isaiah Shavitt Lecturer, Technion, Israel
2013	Computer World Data+ Award
2013	ACS Early Career Award in Theoretical Chemistry
2012	Elected Fellow, American Physical Society
2012	Phillips Distinguished Visitor, Haverford College
2012	Ulam Fellow, Los Alamos National Laboratories
2011	Big Think Delphi Fellowy
2010	MIT Technology Review Young Innovator Under 35 (TR35)
2010	American Chemical Society Hewlett-Packard Outstanding Junior Faculty Award
2010	Everett Mendelsohn Excellence in Mentoring Award
2010	Hascoe Distinguished Lecturer, University of Connecticut
2009	DARPA Young Faculty Award
2009	Camille and Henry Dreyfus Teacher-Scholar
2009	Sloan Research Fellow
2009	Closs Lecturer, University of Chicago
2009	Dow Foundation Distinguished Lecturer, University of California, Santa Barbara

Research

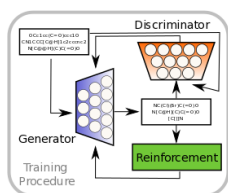
Our group works at the interface of theoretical chemistry with physics, computer science, and applied mathematics. In particular, we are interested in approaches that can be disruptive to the field. We develop and apply quantum computer algorithms for applications in the physical sciences such as the simulation of molecules and materials. We also are working towards the acceleration of molecular discovery by the combination of robotics, artificial intelligence, and high-throughput quantum chemistry to create what we call “materials acceleration platforms” or “self-driving laboratories”. We are a multidisciplinary team composed of chemists, physicists, computer scientists, etc. working both on theory and experiment.



Materials Discovery

Accelerating the discovery of new functional materials through the integration of high-throughput computation, machine learning, and chemical intuition.

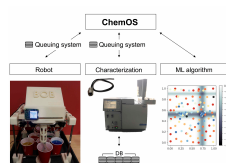
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Machine Learning

Leveraging statistical patterns in chemical data we seek to explore and optimize in chemical space and improve the predictive power of theoretical methods to better match reality.

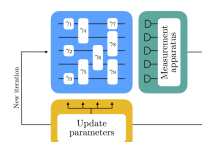
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Self driving chemical laboratories

Orchestrating artificial intelligence and robotic solutions in “self-driving laboratories” to accelerate autonomous material discovery.

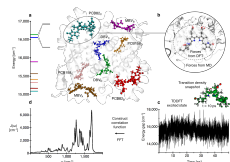
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Quantum Computing

Developing quantum algorithms to access high-accuracy and high-throughput quantum chemical and machine learning calculations.

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Excitonics

Understanding and controlling excited state molecular processes in the condensed phase for light harvesting to logic gates.