Curriculum Vitae

Nike Dattani

Citizenships: Canadian (only)
Birth: Canada (Scarborough, Ontario)

Education:
2005-2009. University of Waterloo. Waterloo, Ontario, Canada (***Bachelor's***, awarded in 2009)
2009-2010. Oxford University. Oxford, England, UK (Pre-Doctoral Student)
2010-2012. Oxford University. Oxford, England, UK (***PhD***, awarded in 2013)
→ **Hetherington Prize** for best Doctoral presentation.

Current Position:
Since 2013. Managing Director of HPQC Labs.

Founder:

Matter Modeling Stack Exchange
https://mattermodeling.stackexchange.com/.

Sponsored community for advanced research-level questions about quantum chemistry and condensed matter physics software.

3700+ members, 1900+ questions, 2600+ answers by:

Geoff Hutchison (lead developer of OpenBabel and AVOGADRO),
Frank Neese (lead developer of ORCA, Director of Max Planck Institute for Chemical Energy)
Anna Krylov (lead developer of Q-Chem),
Todd Martinez (lead developer of TeraChem),
Frank Jensen (author of "Introduction to Computational Chemistry"),
Marcel Swart (Director of IQCC Institute),
Paul Ayers (lead author of HORTON and ChemTools),
Thomas Manz (inventor of DDEC6 atomic charge analysis)
and lead developers of many other software packages.

Supervision and Mentorship of Research Students:

2012-2013: David Mark Wilkins
2014-2014: Staszek Welsh
2014-2014: Nathan Bryans (**now Director of AI at ATB Financial**)
2015-2017: Richard Tanburn (**now a Researcher at Google's DeepMind**)
2015-2016: Emile Okada
2015-2016: Oliver Lunt
2015-2016: Toby Cathcart-Burn
2016-2017: Corinne Duperrouzel
2018-2019: Camilo Sogamoso
2019-2019: Faith Kimongo
2019-2020: Andreas Soteriou
2019-2020: Bhavik Mehta
2021-2021: Nina Tan
2021-2021: Erika Bruulsema
2021-2021: Matthew Charbonneau
2021-2021: Rachelle Fontanilla
2021-2021: Tim Li
2021-2021: Ruby Kong
2021-2021: Nina Tan
2021-2021: Kathryn Waterman
2021-2021: Maya Wei
2021-2021: Tina Yu
2021-2021: Philip Cowan
2021-2022: Yasir Lalmohamed
2022-2022: Qiqi Li
2022-2022: Abdulahad Hussain
2022-2022: Amitkumar Parekh

University Level Teaching (Masters/PhD level):

2019: Concordia University: Special graduate level course "Modeling and Simulations Across Molecular Sciences and Engineering" taught jointly with Matthias Ernzerhof (UMontreal), Sergey Manzhos (INRS), Gilles Peslherbe (Concordia), Heidi Muchall (Concordia), and Guillaume Lamoureaux (Rutgers).
2018: University of Informatics Sciences: Special course on "Quantum Computing".

University Level Teaching (Undergrad level):

2021: University of Waterloo: MATH 135 Mathematical Proofs (2 sections).
2014: Kyoto University: Quantum Molecular Dynamics (guest lecturer)
2013: Oxford University: Quantum Chemistry (2 sections)
2013: Oxford University: Biophysical Chemistry (2 sections)
2013: Oxford University: Statistics for Biochemistry (2 sections)
2012: Oxford University: Materials Modeling (Fourier Series and PDEs)
2012: Oxford University: Quantum Chemistry (2 sections)
2011: Oxford University: Materials Modeling (Fourier Series and PDEs)
2010: Oxford University: Materials Modeling (Fourier Series and PDEs)

Teaching Assistant:
2008: University of Waterloo: PHYS 125 - Physics II for Mechanical Engineering
2008: University of Waterloo: PHYS 122 - Physics II for Physics
2008: University of Waterloo: PHYS 112 - Physics II for Biomedical Science
2008: University of Waterloo: PHYS 111 - Physics I for Kinesiology
2007: University of Waterloo: PHYS 115 - Physics I for Electrical Engineering
2007: University of Waterloo: PHYS 125 - Physics I for Mechanical Engineering

Lab Demonstrator:
2008: University of Waterloo: CHEM 123L - Chemical Reaction Laboratory II
2007: University of Waterloo: CHEM 120L - Chemical Reaction Laboratory I

Teaching for Industry Workshops:

2019: “Advanced Quantum Programming.” Course created entirely by me, with participants ranging from Executives at major banks: “Director of Emerging Technologies” at Barclays Bank (Anthony Macey), to quantum computing start-up companies (Cambridge Quantum Computing), to Chief Technology Officers at artificial intelligence companies (Mario Tsatsos).

Reviewer for large-scale laboratory grants:
2017: QUANTERA: Proposal requesting 900,000 Euro to share between 3 labs over 3 yrs.

Reviewer for Journals (selected):
Journal of Chemical Physics: 4 papers (2014, 2015, 2016, 2018)
Nature: Scientific Reports: 2 papers (2016,2018)
Journal of Quantitative Spectroscopy and Radiative Transfer: 2 papers (2017, 2018)
Chemical Science: 1 paper (2018)
Quantum Information and Computation: 1 paper (2018)
Chemical Physics Letters: 1 paper (2021)
Journal of Physical Chemistry Letters: 1 paper (2017)
Molecular Physics: 1 paper (2018)
Physical Chemistry Research: 1 paper (2017)
Journal of Molecular Spectroscopy: 1 paper (2016)
Physical Review Letters: 1 paper (2013)
Canadian Journal of Physics: 1 paper (2013)

Reviewer for Conference Paper Prizes:
2013: Rao Prize (International Symposium on Molecular Spectroscopy)
2018: Rao Prize (International Symposium on Molecular Spectroscopy)

Grader for Competitions:
2009: British Physics Olympiad

Books:

Nike Dattani. “Quadratization in Discrete Optimization and Quantum Mechanics". 67 Pages, 203 Equations. Preview: https://arxiv.org/abs/1901.04405

Nike Dattani, Camilo Sogamoso “Treatise on Variational Polaron-Transformed Master Equations”. 12 November 2017. 86 pages, 1588 Equations. Completed with assistance of an undergraduate student volunteer (Camilo Sogamoso) from Bogota, Colombia. Preview: https://github.com/HPQC-LABS/FeynDyn/blob/master/Derivations/VPQME.pdf

Most cited papers:

Papers not related to software, with > 75 citations:

1) McCutcheon D., **Dattani N.**, Gauger E., Lovett B., Nazir A. (2011). **Physical Review B** 84 (11), 119903. "General approach to quantum dynamics using a variational master equation: Application to phonon-damped Rabi rotations in quantum dots".

   142 citations on Google scholar.

2) Le Roy R, **Dattani N.**, Coxon J., Ross A., Crozet P., Linton C. (2009). **Journal of Chemical Physics** 131 (20), 204309. "Accurate analytic optentials for Li2(X-state) and Li2(A-state) from 2 to 90 Angstroms".

   110 citations on Google scholar.

3) Wilkins D, **Dattani N**. (2015). **Journal of Chemical Theory and Computation** 11 (7), 3411. "Why quantum coherence is not important in the Fenna-Matthews-Olsen complex".

   88 citations on Google scholar.

Software papers:

1) "OpenMolcas: From source code to insight". (2019). **Journal of Chemical Theory and Computation** 15 (11), 5925.

   288 citations on Google scholar.

2) Kai Guther, Robert J Anderson, Nick S Blunt, Nikolay A Bogdanov, Deidre Cleland, **Nike Dattani**, Werner Dobrautz, Khaldoon Ghanem, Peter Jeszenszki, Niklas Liebermann, Giovanni Li Manni, Alexander Y Lozovoi, Hongjun Luo, Dongxia Ma, Florian Merz, Catherine Overy, Markus Rampp, Pradipta Kumar Samanta, Lauretta R Schwarz, James J Shepherd, Simon D Smart, Eugenio Vitale, Oskar Weser, George H Booth, Ali Alavi. (2020) **Journal of Chemical Physics** 153 (3), 034107. "NECI: N-Electron Configuration Interaction with an emphasis on state-of-the-art stochastic methods".

   22 citations on Google scholar.

3) **Nike Dattani**. (2013). **Computer Physics Communications** 184 (12) 2828. "FeynDyn: A MATLAB program for fast numerical Feynman integral calculations for open quantum system dynamics on GPUs"

   20 citations on Google scholar.

Award-winning papers:

1) **Nike Dattani.** (2015) **Journal of Molecular Spectroscopy** 311, 76-83, "Beryllium monohydride (BeH): Where we are now, after 86 years of spectroscopy" Most-read Publication Award for Second Quarter of 2015

2) Mikhail V Altaisky, Nadezhda N Zolnikova, Natalia E Kaputkina, Victor A Krylov, Yurii E Lozovik, **Nike Dattani** (2016) "Towards a feasible implementation of quantum neural networks using quantum dots" Editor's Pick, and Journal Cover.

Books:

1) **Nike Dattani**. (2019)."Quadratization in discrete optimization and quantum mechanics." **26 citations on Google scholar.**

Publication Authorship Metrics:

of co-authors: 157 (see full list: here).

Co-authors with 10,000+ citations:

1) Don Truhlar (198,425 citations, h-index 185)
2) Hans Lischka (29,983 citations, h-index 75)
3) Per Ake Malmqvist (28,446 citations, h-index 56)
4) Markus Reiher (26,445 citations, h-index 78)
5) Laura Galgiardi (24,461 citations, h-index 55)
6) Roland Lindh (22,372 citations, h-index 73)
7) David Feller (20,784 citations, h-index 74)
8) Erin Johnson (19,622 citations, h-index 45)
9) Ludwik Adamowicz (18,172 citations, h-index 65)
10) Garnet Chan (16,171 citations, h-index 66)
11) Bob Le Roy (12,985 citations, h-index 54)
12) Ali Alavi (12,353 citations, h-index 59
13) Cyrus Umrigar (10,006 citations, h-index 52)