

# Curriculum Vitae

Nike Dattani

**Citizenships:** Canadian (only)

**Birth:** Canada (Scarborough, Ontario)

## **Education:**

2005-2009. University of Waterloo. Waterloo, Ontario, Canada (**Bachelors**, 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 Lamoureux](#) (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.** "Quadratrization 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 potentials for Li<sub>2</sub>(X-state) and Li<sub>2</sub>(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, Khaldoun Ghanem, Peter Jeszenszki, Niklas Liebermann, Giovanni Li Manni, Alexander Y Lozovoi, Hongjun Luo, Dongxia Ma, Florian Merz, Catherine Overy, Markus Rampp, Pradipta Kumar Samanta, Laretta 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). **Harvard University Press**. “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 Galgardi](#) (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)