Robert Pollice
Stratingh Institute for Chemistry, University of Groningen
Nijenborgh 4, 9747 AG Groningen, The Netherlands
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Research Interests

Artificial Molecular Design, Catalysis, Organic Chemistry, Machine Learning, Cheminformatics, Reaction Mechanisms, Physical Organic Chemistry, Molecular Interactions

Education

2015 – 2019 **PhD Physical Organic Chemistry, ETH Zurich**
Research Advisor: Professor Dr. Peter Chen
Thesis: "London Dispersion in Molecular Systems"
2013 – 2015 **MSc Technical Chemistry, TU Wien, with distinction**
Research Advisor: Professor Dr. Michael Schnürch
Thesis: "Mechanistic Investigations of C-H Activation Reactions"
2010 – 2013 **BSc Technical Chemistry, TU Wien, with distinction**

Professional Experience

2022 – **Assistant Professor for Computer-Aided Organic Synthesis, University of Groningen**
2019 – 2022 **Postdoctoral Fellow, Prof. Dr. Alán Aspuru-Guzik, University of Toronto**

Teaching Experience

2018 Teaching Assistant for Physical Organic Chemistry, ETH Zurich
2015 – 2016 Teaching Assistant for Practical Course Organic Chemistry, ETH Zurich
2014 Teaching Assistant for Synthesis Laboratory Course, TU Wien

Awards and Fellowships

2022 Selected Participant of the 71st Lindau Nobel Laureate Meeting in 2022
2021 Selected Participant of the 70th Lindau Nobel Laureate Meeting in 2021
2020 Finalist of the Reaxys PhD Prize 2020
Prix Schläfli for the Best Swiss Dissertation in Chemistry
Silver Medal of ETH Zurich for Outstanding Doctoral Thesis
3rd place at the Lindau Online Sciathon 2020
2019 Swiss National Science Foundation (SNF) Postdoc.Mobility Fellowship
2017 Gordon Research Conferences Scholarship
2016 Chemistry Travel Award by the SCNAT, the SCS and the SSFC
2015 State Prize for the master thesis by the Austrian Federal Ministry of Science,

Research and Economy
2014 Sponsorship Prize for the master thesis by the Austrian Chemical Society (GÖCH)
Oxford University Press Achievement in Chemistry Prize
2010 Gold medal (4th place) at the 42nd International Chemistry Olympiad in Tokyo, Japan
2009 Gold medal (13th place) at the 41st International Chemistry Olympiad in Cambridge, United Kingdom

Research Output

A. Publications (# indicates equal contributions, * indicates corresponding authorship)

26. R. A. Vargas-Hernández*, K. Jorner, **R. Pollice**, A. Aspuru-Guzik:
"Inverse molecular design and parameter optimization with Hückel theory using automatic differentiation"
J. Chem. Phys **2023**. In Press. https://doi.org/10.1063/5.0137103

25. A. Lo*, **R. Pollice***, A. Nigam, A. D. White, M. Krenn, A. Aspuru-Guzik*:
"Recent advances in the Self-Referencing Embedding Strings (SELFIES) library"
arXiv **2023**. Preprint. https://doi.org/10.48550/arXiv.2302.03620

24. T. C. Wu#, A. A. Granda#, K. Hotta, S. A. Yazdani, **R. Pollice**, J. Vestfrid, H. Hao, C. Lavigne, M. Seifrid, N. Angello, F. Bencheikh, J. E. Hein, M. Burke, C. Adachi, A. Aspuru-Guzik*:
"A Materials Acceleration Platform for Organic Laser Discovery"
Adv. Mater. **2022**. In Press. https://doi.org/10.1002/adma.202207070

23. C. Lavigne, G. d. P. Gomes#,*, **R. Pollice**#,*, A. Aspuru-Guzik*:
"Guided Discovery of Chemical Reaction Pathways with Imposed Activation"
Chem. Sci. **2022**. *13*, 13857 – 13871. https://doi.org/10.1039/D2SC05135D

22. M. Krenn*, Q. Ai, S. Barthel, N. Carson, A. Frei, N. C. Frey, P. Friederich, T. Gaudin, A. A. Gayle, K. M. Jablonka, R. F. Lameiro, D. Lemm, A. Lo, S. M. Moosavi, J. M. Nápoles-Duarte, A. Nigam, **R. Pollice**, K. Rajan, U. Schatzschneider, P. Schwaller, M. Skreta, B. Smit, F. Strieth-Kalthoff, C. Sun, G. Tom, G. F. von Rudorff, A. Wang, A. White, A. Young, R. Yu, A. Aspuru-Guzik*:
"SELFIES and the future of molecular string representations"
Patterns **2022**, *3*, 100588. https://doi.org/10.1016/j.patter.2022.100588

21. M. Krenn*, **R. Pollice**, S. Y. Guo, M. Aldeghi, A. Cervera-Lierta, P. Friederich, G. d. P. Gomes, F. Häse, A. Jinich, A. Nigam, Z. Yao, A. Aspuru-Guzik*:
"On scientific understanding with artificial intelligence"
Nat. Rev. Phys. **2022**, *4*, 761 – 769. https://doi.org/10.1038/s42254-022-00518-3

20. A. Nigam, **R. Pollice***, G. Tom, K. Jorner, L. A. Thiede, A. Kundaje, A. Aspuru-Guzik:
"Tartarus: A Benchmarking Platform for Realistic And Practical Inverse Molecular Design"
arXiv **2022**. Preprint. https://doi.org/10.48550/arXiv.2209.12487

19. M. Seifrid, **R. Pollice**, A. Aguilar-Granda, Z. M. Chan, K. Hotta, C. T. Ser, J. Vestfrid, T. C. Wu, A. Aspuru-Guzik*:
"Autonomous Chemical Experiments: Challenges and Perspectives on Establishing a

Self-Driving Lab"
Acc. Chem. Res. **2022**, *55*, 2454 – 2466.
https://doi.org/10.1021/acs.accounts.2c00220

18. A. Nigam[#], **R. Pollice**[#], A. Aspuru-Guzik*:
"Parallel Tempered Genetic Algorithm Guided by Deep Neural Networks for Inverse Molecular Design"
Digital Discovery **2022**, *1*, 390 – 440. https://doi.org/10.1039/D2DD00003B

17. T. Gensch[#,*], G. d. P. Gomes[#], P. Friederich[#], E. Peters, T. Gaudin, **R. Pollice**, K. Jorner, A. Nigam, M. Lindner-D'Addario, M. S. Sigman*, A. Aspuru-Guzik*:
"A Comprehensive Discovery Platform for Organophosphorus Ligands for Catalysis"
J. Am. Chem. Soc. **2022**, *144*, 1205 – 1217. https://doi.org/10.1021/jacs.1c09718

16. A. Nigam, **R. Pollice**, M. F. D. Hurley, R. J. Hickman, M. Aldeghi, N. Yoshikawa, S. Chithrananda, V. A. Voelz, A. Aspuru-Guzik*:
"Assigning Confidence to Molecular Property Prediction"
Expert Opin. Drug Discov. **2021**, *19*, 1009 – 1023.
https://doi.org/10.1080/17460441.2021.1925247

15. A. Nigam, **R. Pollice**, M. Krenn, G. d. P. Gomes, A. Aspuru-Guzik*:
"Beyond Generative Models: Superfast Traversal, Optimization, Novelty, Exploration and Discovery (STONED) Algorithm for Molecules using SELFIES"
Chem. Sci. **2021**, *12*, 7079 – 7090. https://doi.org/10.1039/D1SC00231G

14. **R. Pollice**, P. Friederich, C. Lavigne, G. d. P. Gomes, A. Aspuru-Guzik*:
"Organic Molecules with Inverted Gaps between First Excited Singlet and Triplet States and Appreciable Fluorescence Rates"
Matter **2021**, *4*, 1654 – 1682. https://doi.org/10.1016/j.matt.2021.02.017

13. **R. Pollice**, G. d. P. Gomes, M. Aldeghi, R. J. Hickman, M. Krenn, C. Lavigne, M. Lindner-D'Addario, A. Nigam, C. T. Ser, Z. Yao, A. Aspuru-Guzik*:
"Data-Driven Strategies for Accelerated Materials Design"
Acc. Chem. Res. **2021**, *54*, 849 – 860. https://doi.org/10.1021/acs.accounts.0c00785

12. G. d. P. Gomes[#], **R. Pollice**[#], A. Aspuru-Guzik*:
"Navigating through the Maze of Homogeneous Catalyst Design with Machine Learning"
Trends Chem. **2021**, *3*, 96 – 110. https://doi.org/10.1016/j.trechm.2020.12.006

11. **R. Pollice**, F. Fleckenstein, I. G. Shenderovich, P. Chen*:
"Compensation of London Dispersion in the Gas Phase and in Aprotic Solvents"
Angew. Chem. Int. Ed. **2019**, *58*, 14281 – 14288.
https://doi.org/10.1002/anie.201905436

10. **R. Pollice**, P. Chen*:
"A Universal Quantitative Descriptor of the Dispersion Interaction Potential"
Angew. Chem. Int. Ed. **2019**, *58*, 9758 – 9769. https://doi.org/10.1002/anie.201905439

9. **R. Pollice***:
"A General Fitting Function to Estimate Apparent Reaction Orders of Kinetic Profiles"
ChemRxiv **2019**. Preprint. https://doi.org/10.26434/chemrxiv.7885760.v1

8. D. Schönbauer, M. Spettel, **R. Pollice**, E. Pittenauer, M. Schnürch*:
"Investigations of the generality of quaternary ammonium salts as alkylating agents in direct C-H alkylation reactions: solid alternatives for gaseous olefins"
Org. Biomol. Chem. **2019**, *17*, 4024 – 4030. https://doi.org/10.1039/C9OB00243J

7. **R. Pollice**, P. Chen*:
"Origin of the Immiscibility of Alkanes and Perfluoroalkanes"
J. Am. Chem. Soc. **2019**, *141*, 3489 – 3506. https://doi.org/10.1021/jacs.8b10745

6. M. Anschuber, **R. Pollice**, M. Schnürch*:
"Rhodium-catalyzed Direct Alkylation of Benzylic Amines using Alkyl Bromides"
Monatsh. Chem. **2019**, *150*, 127 – 138. https://doi.org/10.1007/s00706-018-2305-9

5. **R. Pollice**, M. Bot, I. J. Kobylianskii, I. G. Shenderovich, P. Chen*:
"Attenuation of London Dispersion in Dichloromethane Solutions"
J. Am. Chem. Soc. **2017**, *139*, 13126 – 13140. https://doi.org/10.1021/jacs.7b06997

4. M. Spettel, **R. Pollice**, M. Schnürch*:
"Quaternary Ammonium Salts as Alkylating Reagents in C–H Activation Chemistry"
Org. Lett. **2017**, *19*, 4287 – 4290. https://doi.org/10.1021/acs.orglett.7b01946

3. **R. Pollice**, M. Schnürch*:
"Expansion of the Concept of Nonlinear Effects in Catalytic Reactions Beyond Asymmetric Catalysis"
Chem. Eur. J. **2016**, *22*, 5637 – 5642. https://doi.org/10.1002/chem.201504970

2. **R. Pollice**, M. Schnürch*:
"Investigations into the Kinetic Modelling of the Direct Alkylation of Benzylic Amines: Dissolution of K_2CO_3 is responsible for the Observation of an Induction Period"
J. Org. Chem. **2015**, *80*, 8268 – 8274. https://doi.org/10.1021/acs.joc.5b01335

1. **R. Pollice**, N. Dastbaravardeh, N. Marquise, M.D. Mihovilovic, M. Schnürch*:
"Mechanistic and Kinetic Studies of the Direct Alkylation of Benzylic Amines – A Formal C(sp^3)-H Activation Proceeds Actually via a C(sp^2)-H Activation Pathway"
ACS Catal. **2015**, *5*, 587 – 595. https://doi.org/10.1021/cs501924c

B. Patents

1. **R. Pollice**, P. Friederich, C. Lavigne, G. d. P. Gomes, A. Aspuru-Guzik:
"Organic Molecule Light Emitters"
PCT/CA2021/051423, filed 08.10.**2021**, Patent pending.

C. Conferences

2022 **R. Pollice**:
"Design of Organic Molecules with Inverted Singlet-Triplet Gaps"
Invited Lecture: The 7th International TADF Workshop, Virtual; 1.12.2022 – 2.12.2022

R. Pollice, A. Nigam, A. Aspuru-Guzik:
"JANUS: Parallel Tempered Genetic Algorithm Guided by Deep Neural Networks for Inverse Molecular Design"
Contributed Lecture: ACS Spring 2022, San Diego, CA, USA; 20.03.2022 – 24.03.2022

2021 **R. Pollice**, P. Friederich, C. Lavigne, G. d. P. Gomes, A. Aspuru-Guzik:
"Organic Molecules with Inverted Gaps between First Excited Singlet and Triplet States and Appreciable Fluorescence Rates"
Contributed Lecture: 49th Physical Organic Minisymposium, Waterloo, ON, Canada; 13.11.2021 – 14.11.2021

R. Pollice, P. Friederich, C. Lavigne, G. d. P. Gomes, A. Aspuru-Guzik:
"Organic Molecules with Inverted Gaps between First Excited Singlet and Triplet States and Appreciable Fluorescence Rates"
Poster: SCS Fall Meeting 2021, Virtual; 10.09.2021

R. Pollice, P. Friederich, C. Lavigne, G. d. P. Gomes, A. Aspuru-Guzik:
"Organic Molecules with Inverted Gaps between First Excited Singlet and Triplet States and Appreciable Fluorescence Rates"
Contributed Lecture: ACS Fall 2021, Atlanta, GA, USA; 22.08.2021 – 26.08.2021

A. Nigam, **R. Pollice**, M. Krenn, G. d. P. Gomes, A. Aspuru-Guzik:
"Efficient Interpolation and Exploration of the Chemical Space with STONED SELFIES"
Contributed Lecture: ACS Fall 2021, Atlanta, GA, USA; 22.08.2021 – 26.08.2021

2020 **R. Pollice**, C. Lavigne, G. d. P. Gomes, A. Aspuru-Guzik:
"Automatic Discovery of Chemical Reactions Using Imposed Activation"
Contributed Lecture: 48th Physical Organic Minisymposium, Kingston, ON, Canada; 07.11.2020 – 08.11.2020

R. Pollice, P. Chen:
"London Dispersion in Molecular Systems"
Poster: Reaxys PhD Prize Symposium 2020, Virtual; 30.09.2020 – 02.10.2020

2019 **R. Pollice**, P. Chen:
"A Universal Quantitative Descriptor of the Dispersion Interaction Potential"
Contributed Lecture: 47th Physical Organic Minisymposium, York, ON, Canada; 01.11.2019 – 03.11.2019

R. Pollice:
"Reaction Progress Kinetic Analysis By Direct Analysis of Concentration-Time Profiles";
Contributed Lecture: 21st European Symposium on Organic Chemistry, Vienna, Austria; 14.07.2019 – 18.07.2019;

R. Pollice, P. Chen:
"A Universal Descriptor of Dispersive Interaction Potential"
Contributed Lecture: Physical Organic Chemistry Gordon Research Conference, Holderness, NH, USA; 23.06.2019 – 28.06.2019

2018 **R. Pollice**, P. Chen:
"Trends in Intermolecular Dispersion Explain Differences in Properties of Alkanes and Perfluoroalkanes"
Poster: 22nd International Symposium on Fluorine Chemistry, Oxford, United Kingdom; 22.07.2018 – 27.07.2018

R. Pollice, P. Chen:
"Reaction Progress Kinetic Analysis By Direct Analysis of Concentration-Time Profiles"
Contributed Lecture: International Symposium on Reactive Intermediates and Unusual Molecules, Ascona, Switzerland; 15.07.2018 – 20.07.2018

R. Pollice, P. Chen:
"Competing Bond Dissociation Between Covalent Bonds and A Dispersion-Supported Hydrogen Bond"
Poster: International Symposium on Reactive Intermediates and Unusual Molecules, Ascona, Switzerland; 15.07.2018 – 20.07.2018

R. Pollice, P. Chen:
"Reaction Progress Kinetic Analysis By Direct Analysis of Concentration-Time Profiles";
Poster: Reaction Mechanisms Conference, Vancouver, BC, Canada; 10.06.2018 – 13.06.2018

2017 **R. Pollice**, I. Shenderovich, P. Chen:
"Attenuation of London Dispersion in Dichloromethane Solutions"
Poster: Physical Organic Chemistry Gordon Research Conference, Holderness, NH, USA; 25.06.2017 – 30.06.2017

2016 **R. Pollice**, M. Schnürch:
"Expansion of the Concept of Nonlinear Effects in Catalytic Reactions Beyond Asymmetric Catalysis"
Poster: 15th Belgian Organic Synthesis Symposium, Antwerp, Belgium; 10.07.2016 – 15.07.2016

2015 **R. Pollice**, M. Schnürch:
"Investigations into the Kinetic Modelling of the Direct Alkylation of Benzylic Amines: Potassium carbonate is responsible for the Observation of an Induction Period"
Poster: 18th IUPAC International Symposium on Organometallic Chemistry Directed Towards Organic Synthesis, Sitges – Barcelona, Spain; 28.06.2015 – 02.07.2015

2014 **R. Pollice**, M. Schnürch, M.D. Mihovilovic:
"Mechanistic insight into a Rh(I)-catalyzed C-H alkylation of benzylic amines – A seemingly sp^3-sp^3 coupling proceeding via an sp^2-sp^2 mechanism"
Poster: 2nd International Symposium on C-H Activation, Rennes; 30.06.2014 – 03.07.2014

D. Invited Talks

2023 Zernike Institute for Advanced Materials Colloquium, University of Groningen
2022 Prix-Schläfli Mini-Symposium, University of Geneva

Prix-Schläfli Mini-Symposium, University of Bern
Prix-Schläfli Mini-Symposium, University of Zurich
Prix-Schläfli Mini-Symposium, ETH Zurich
CHAIR Virtual Seminar on AI

E. Services

- Co-Chair of Gordon Research Seminar Physical Organic Chemistry 2023
- Reviewer: SLAS Technology, ACS Catalysis, F1000Research, Machine Learning: Science and Technology, Wiley Interdisciplinary Reviews: Computational Molecular Science, Beilstein Journal of Organic Chemistry, Nature Computational Science, Journal of Solution Chemistry, Chemical Science, Advanced Science, Journal of Chemical Theory and Computation, Dalton Transactions, Advanced Theory and Simulations, Journal of Materials Chemistry A, Journal of Physical Organic Chemistry, Materials Advances, Nature Reviews, The Journal of Organic Chemistry, Chem, Journal of Chemical Information and Modeling, Journal of the American Chemical Society, Organic Process Research & Development, Angewandte Chemie, Nature Synthesis, Measurement Science and Technology, Patterns
- Behringer Simon Lecture committee member 2015 – 2017, chair 2016 – 2017, invited, organized and hosted lectures of both academic and industrial speakers in the field of chemistry

F. Outreach

- Contributor to https://researchseminars.org/ for establishing an open web database of research seminars
- Member of the Society of the Friends of the Austrian Chemistry Olympiad since 2008, mentored Chemistry Olympiad participants, conducted public presentations for middle and high school students, delivered a seminar about personal career path for other members
- Weekly highlighting of chemistry publications via #RobSelects on the social media platforms Twitter and Mastodon since 2020