Robert Pollice

Research interests

Current technological advances in computing and robotics are revolutionizing almost everything around us, from industrial manufacturing to the entertainment industry. The Pollice group seeks to implement these technological advances in the realm of organic chemistry to tackle a problem that has fascinated chemists for more than two centuries, the design of new catalysts. Our group will combine automated experimentation with computational screening and machine learning to accelerate the development of catalytic organic reactions. To achieve that, we welcome scientists from various fields to build an interdisciplinary team.
Just like a researcher documents the outcome of previous experiments and uses this information to plan subsequent ones, some of the most efficient optimization algorithms rely on continuous feedback loops using the data collected most efficiently. Hence, we interface computer algorithms tasked with finding the best catalyst for a chemical reaction with chemistry labs. Using the data that we will collect during closed-loop catalyst optimization, our group will integrate, refine, and benchmark molecular design algorithms and use them to create new molecular catalysts.

Employment

Research outputs

Computational Investigations of the Detailed Mechanism of Reverse Intersystem Crossing in Inverted Singlet-Triplet Gap Molecules
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Ultrafast Computational Screening of Molecules with Inverted Singlet-Triplet Energy Gaps Using the Pariser-Parr-Pople Semiempirical Quantum Chemistry Method
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Chromium delivers twice
Hovorka, H. & Pollice, R., Nov-2023, In: Nature synthesis. 2, p. 1012–1013 2 p.

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Lo, A., Pollice, R., Nigam, A. K., White, A. D., Krenn, M. & Aspuru-Guzik, A., 1-Aug-2023, In: Digital Discovery. 2, 4, p. 897-908 12 p.

Inverse molecular design and parameter optimization with Hückel theory using automatic differentiation
Vargas-Hernández, R. A., Jorner, K., Pollice, R. & Aspuru-Guzik, A., 14-Mar-2023, In: Journal of Chemical Physics. 158, 10, 17 p., 104801.

A Materials Acceleration Platform for Organic Laser Discovery
Wu, T. C., Aguilar-Granda, A., Hotta, K., Yazdani, S. A., Pollice, R., Vestfrid, J., Hao, H., Lavigne, C., Seifrid, M., Angello, N., Bencheikh, F., Hein, J. E., Burke, M., Adachi, C. & Aspuru-Guzik, A., 9-Feb-2023, In: Advanced materials. 35, 6, 9 p., 2207070.

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Guided discovery of chemical reaction pathways with imposed activation
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On scientific understanding with artificial intelligence
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Activities

Chem (Journal)

Robert Pollice (Peer reviewer)
2022 → …

Journal of chemical information and modeling (Journal)
Robert Pollice (Peer reviewer)
2022 → …

Journal of the American Chemical Society (Journal)
Robert Pollice (Peer reviewer)
2022 → …

Materials Advances (Journal)
Robert Pollice (Peer reviewer)
2022 → …

Organic Process Research & Development (Journal)
Robert Pollice (Peer reviewer)
2022 → …

The Journal of Organic Chemistry (Journal)
Robert Pollice (Peer reviewer)
2022 → …

Advanced science (Journal)
Robert Pollice (Peer reviewer)
2021 → …

Advanced theory and simulations (Journal)
Robert Pollice (Peer reviewer)
2021 → …

Chemical Science (Journal)
Robert Pollice (Peer reviewer)
2021 → …

Dalton Transactions (Journal)
Robert Pollice (Peer reviewer)
2021 → …

Journal of Chemical Theory and Computation (Journal)
Robert Pollice (Peer reviewer)
2021 → …

Journal of Materials Chemistry A (Journal)
Robert Pollice (Peer reviewer)
2021 → …

Journal of physical organic chemistry (Journal)
Robert Pollice (Peer reviewer)
2021 → …

Journal of Solution Chemistry (Journal)
Robert Pollice (Peer reviewer)
2021 → …

Materials Advances (Journal)
Robert Pollice (Peer reviewer)
2021 → …

Nature Computational Science (Journal)
Robert Pollice (Peer reviewer)
2021 → …

Nature reviews chemistry (Journal)
Robert Pollice (Peer reviewer)
2021 → …

Beilstein Journal of Organic Chemistry (Journal)
Robert Pollice (Peer reviewer)
2020 → …

F1000Research (Journal)
Robert Pollice (Peer reviewer)
2020 → …

Machine Learning: Science and Technology (Journal)
Robert Pollice (Peer reviewer)
2020 → …

Wiley Interdisciplinary Reviews: Computational Molecular Science (Journal)
Robert Pollice (Peer reviewer)
2020 → …

ACS Catalysis (Journal)
Robert Pollice (Peer reviewer)
2019 → …

SLAS Technology (Journal)
Robert Pollice (Peer reviewer)
2019 → …