



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

Application of established computational techniques to identify potential SARS-CoV-2 Nsp14-MTase inhibitors in low data regimes

Nigam, A. K., Hurley, M. F. D., Li, F., Konkořová, E., Klíma, M., Trylčová, J., Pollice, R., Çinaroğlu, S. S., Levin-Konigsberg, R., Handjaya, J., Schapira, M., Chau, I., Perveen, S., Ng, H. L., Kaniskan, H. Ü., Han, Y., Singh, S., Gorgulla, C., Kundaje, A. & Jin, J. & 6 others, Voelz, V. A., Weber, J., Nencka, R., Boura, E., Vedadi, M. & Aspuru-Guzik, A., 1-Jul-2024, In: Digital Discovery. 3, 7, p. 1327-1341 15 p., d4dd00006d.

The Fe-MAN Challenge: Ferrates-Microkinetic Assessment of Numerical Quantum Chemistry

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Delocalized, asynchronous, closed-loop discovery of organic laser emitters

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Computational Investigations of the Detailed Mechanism of Reverse Intersystem Crossing in Inverted Singlet-Triplet Gap Molecules

Valverde, D., Ser, C. T., Ricci, G., Jorner, K., Pollice, R., Aspuru-Guzik, A. & Olivier, Y., 10-May-2024, (E-pub ahead of print) In: ACS Applied Materials & Interfaces. 11 p., 4c04347.

A guidebook for sustainability in laboratories

Freese, T., Kat, R., Lanooij, S. D., Böllersen, T. C., De Roo, C. M., Elzinga, N., Beatty, M., Setz, B., Weber, R. R., Malta, I., Gandek, T. B., Krikken, A. M., Fodran, P., Pollice, R. & Lerch, M. M., 25-Apr-2024, (E-pub ahead of print) ChemRxiv. 76 p.

Ultrafast Computational Screening of Molecules with Inverted Singlet-Triplet Energy Gaps Using the Pariser-Parr-Pople Semiempirical Quantum Chemistry Method

Jorner, K., Pollice, R., Lavigne, C. & Aspuru-Guzik, A., 28-Mar-2024, In: Journal of Physical Chemistry A. 128, 12, p. 2445-2456 12 p.

Rational design of organic molecules with inverted gaps between the first excited singlet and triplet
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Activities

Chem (Journal)

Pollice, R. (Peer reviewer)
2022 → ...

Journal of chemical information and modeling (Journal)

Pollice, R. (Peer reviewer)
2022 → ...

Journal of the American Chemical Society (Journal)

Pollice, R. (Peer reviewer)
2022 → ...

Materials Advances (Journal)

Pollice, R. (Peer reviewer)
2022 → ...

Organic Process Research & Development (Journal)

Pollice, R. (Peer reviewer)
2022 → ...

The Journal of Organic Chemistry (Journal)

Pollice, R. (Peer reviewer)
2022 → ...

Advanced science (Journal)

Pollice, R. (Peer reviewer)
2021 → ...

Advanced theory and simulations (Journal)

Pollice, R. (Peer reviewer)
2021 → ...

Chemical Science (Journal)

Pollice, R. (Peer reviewer)
2021 → ...

Dalton Transactions (Journal)

Pollice, R. (Peer reviewer)
2021 → ...

Journal of Chemical Theory and Computation (Journal)

Pollice, R. (Peer reviewer)

2021 → ...

Journal of Materials Chemistry A (Journal)

Pollice, R. (Peer reviewer)

2021 → ...

Journal of physical organic chemistry (Journal)

Pollice, R. (Peer reviewer)

2021 → ...

Journal of Solution Chemistry (Journal)

Pollice, R. (Peer reviewer)

2021 → ...

Materials Advances (Journal)

Pollice, R. (Peer reviewer)

2021 → ...

Nature Computational Science (Journal)

Pollice, R. (Peer reviewer)

2021 → ...

Nature reviews chemistry (Journal)

Pollice, R. (Peer reviewer)

2021 → ...

Beilstein Journal of Organic Chemistry (Journal)

Pollice, R. (Peer reviewer)

2020 → ...

F1000Research (Journal)

Pollice, R. (Peer reviewer)

2020 → ...

Machine Learning: Science and Technology (Journal)

Pollice, R. (Peer reviewer)

2020 → ...

Wiley Interdisciplinary Reviews: Computational Molecular Science (Journal)

Pollice, R. (Peer reviewer)

2020 → ...

ACS Catalysis (Journal)

Pollice, R. (Peer reviewer)

2019 → ...

SLAS Technology (Journal)

Pollice, R. (Peer reviewer)

2019 → ...