Open Access Article. Published on 03 December 2025. Downloaded on 2/27/2026 8:14:31 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

Digital Discovery

rsc.li/digitaldiscovery

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

IN THIS ISSUE

ISSN 2635-098X CODEN DDIIAI 4(12) 3415–3830 (2025)

Cover
See Olexandr Isayev *et al.*, pp. 3445–3454. Image reproduced by permission of Ekaterina Ustiuzhanina from Olexandr Isayev *et al.*, *Digital Discovery*, 2025, **4**, 3445. Image by Ekaterina Ustiuzhanina.

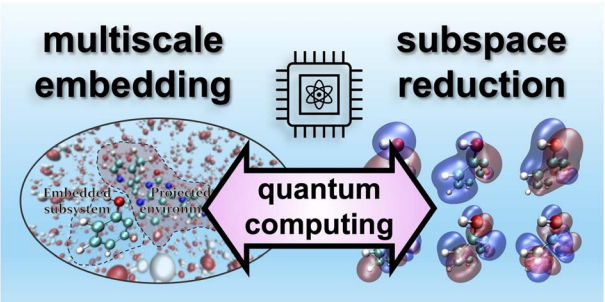
Inside cover
See Ge Lei and Samuel J. Cooper, pp. 3455–3465. Image reproduced by permission of Ge Lei and Samuel J. Cooper from *Digital Discovery*, 2025, **4**, 3455. Image created with the use of Google Gemini and Adobe Photoshop Generative Fill.

PERSPECTIVE

3427

Extending quantum computing through subspace, embedding and classical molecular dynamics techniques

Thomas M. Bickley, Angus Mingare, Tim Weaving, Michael Williams de la Bastida, Shunzhou Wan, Martina Nibbi, Philipp Seitz, Alexis Ralli, Peter J. Love, Minh Chung, Mario Hernández Vera, Laura Schulz and Peter V. Coveney*

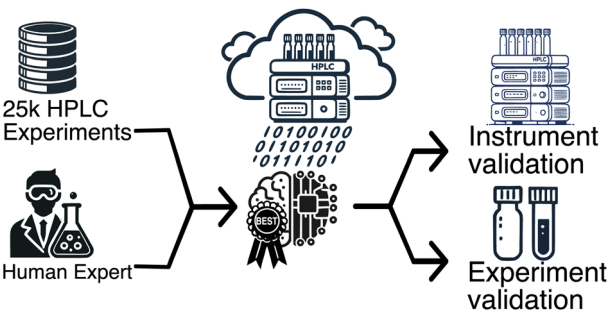


PAPERS

3445

Machine learning anomaly detection of automated HPLC experiments in the cloud laboratory

Filipp Gusev, Benjamin C. Kline, Ryan Quinn, Anqin Xu, Ben Smith, Brian Frezza and Olexandr Isayev*



ROYAL SOCIETY OF CHEMISTRY

Royal Society of Chemistry approved training courses

Explore your options.
Develop your skills.
Discover learning that suits you.

Courses in the classroom, the lab, or online

Find something for every stage of your professional development. Search our database by:

- subject area
- location
- event type
- skill level

Members **get at least 10% off**

Visit **rsc.li/cpd-training**

SAVE 10%

Registered charity number: 207890

This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

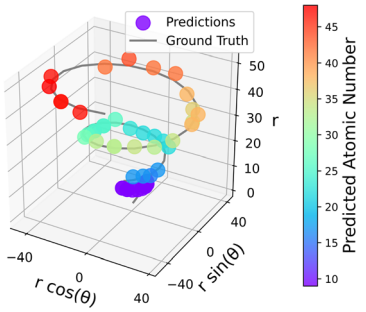
Open Access Article. Published on 03 December 2025. Downloaded on 2/27/2026 8:14:31 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

PAPERS

3455

Do Llamas understand the periodic table?

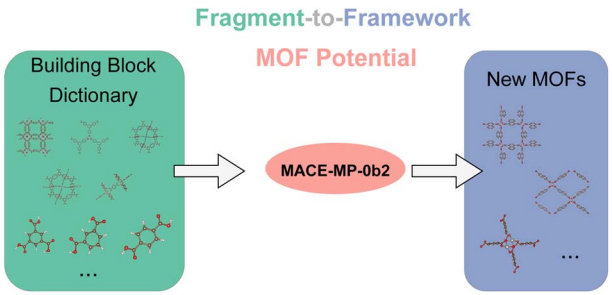
Ge Lei* and Samuel J. Cooper



3466

FFLAME: a fragment-to-framework learning approach for MOF potentials

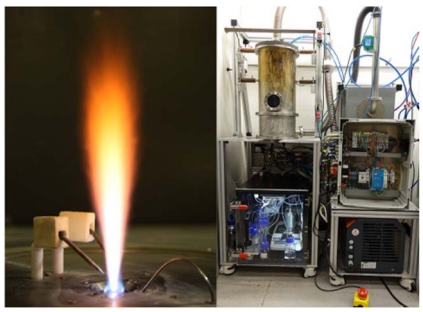
Xiaoqi Zhang, Yutao Li, Xin Jin and Berend Smit*



3478

An automated platform for "on-demand" high-speed catalyst synthesis by flame spray pyrolysis

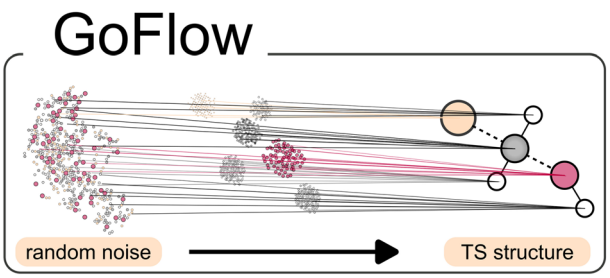
Konstantin M. Engel, Patrik O. Willi, Robert N. Grass and Wendelin J. Stark*



3492

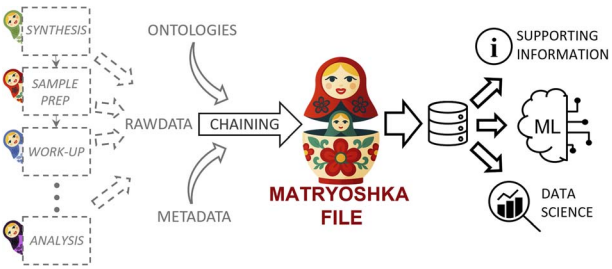
GoFlow: efficient transition state geometry prediction with flow matching and E(3)-equivariant neural networks

Leonard Galustian, Konstantin Mark, Johannes Karwounopoulos, Maximilian P.-P. Kovar and Esther Heid*



Open Access Article. Published on 03 December 2025. Downloaded on 2/27/2026 8:14:31 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

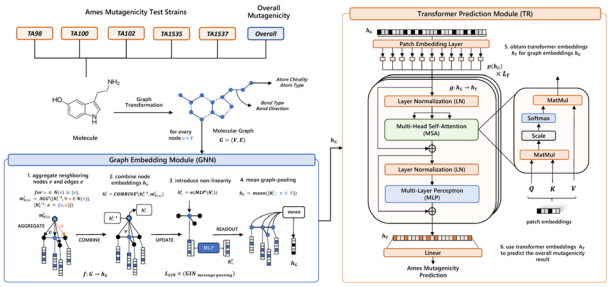
3502



A FAIR research data infrastructure for high-throughput digital chemistry

Alice Gauthier, Laure Vancauwenberghe, Jean-Charles Cousty,* Cyril Matthey-Doret, Robin Franken, Sabine Maennel, Pascal Miéville and Oksana Riba Grognuz

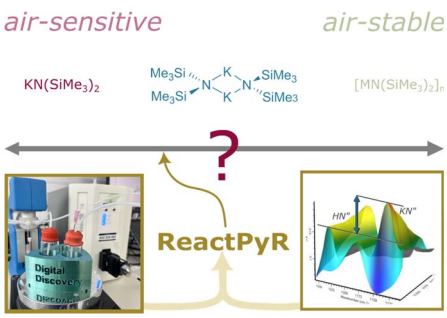
3515



Advancing mutagenicity predictions in drug discovery with an explainable few-shot deep learning framework

Luis H. M. Torres,* Sofia M. da Silva, Joel P. Arrais, Catarina Pimentel and Bernardete Ribeiro

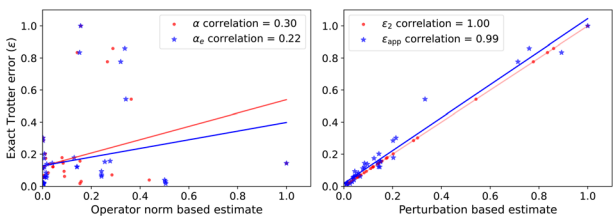
3533



ReactPyR: a python workflow for ReactIR allows for quantification of the stability of sensitive compounds in air

Nicola L. Bell,* Emanuele Berardi, Marina Gladkikh, Richard Drummond Turnbull and Freya Turton

3540



Estimating Trotter approximation errors to optimize Hamiltonian partitioning for lower eigenvalue errors

Shashank G. Mehendale, Luis A. Martínez-Martínez, Prathami Divakar Kamath and Artur F. Izmaylov*

 This journal is © The Royal Society of Chemistry 2025

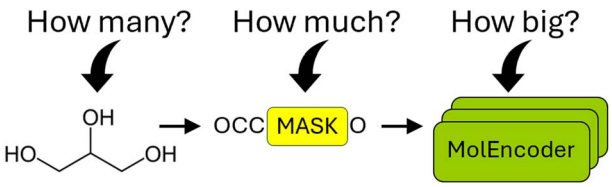
Open Access Article. Published on 03 December 2025. Downloaded on 2/27/2026 8:14:31 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

PAPERS

3552

MolEncoder: towards optimal masked language modeling for molecules

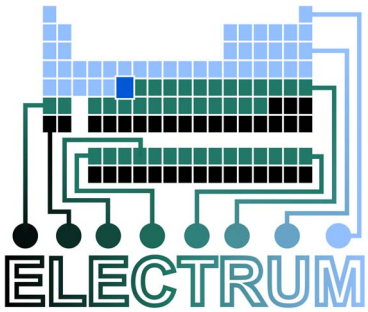
Fabian P. Krüger,* Nicklas Österbacka, Mikhail Kabeshov, Ola Engkvist and Igor Tetko



3567

ELECTRUM: an electron configuration-based universal metal fingerprint for transition metal compounds

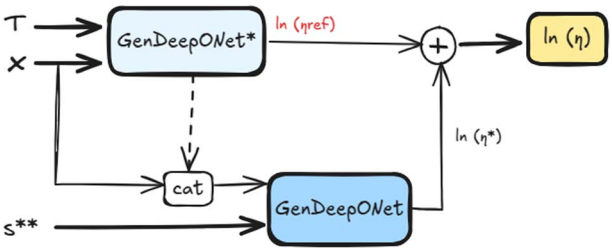
Markus Orsi* and Angelo Frei*



3578

Generalized DeepONets for viscosity prediction using learned entropy scaling references

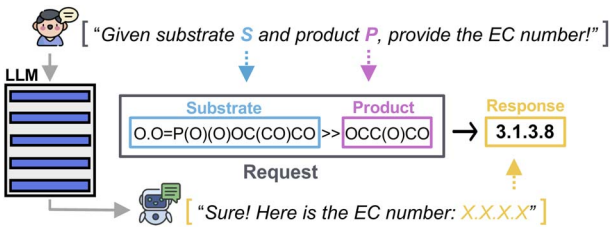
Maximiliam Fleck,* Marcelle B. M. Spera, Samir Darouich, Timo Klenk and Niels Hansen*



3588

Leveraging large language models for enzymatic reaction prediction and characterization

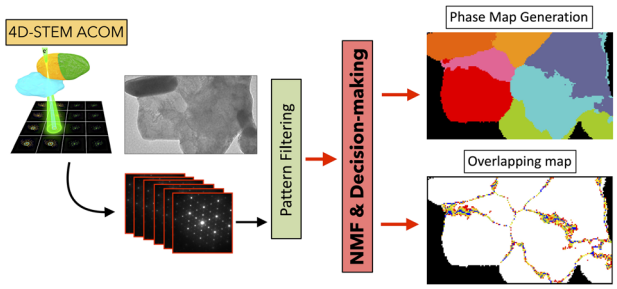
Lorenzo Di Fruscia and Jana M. Weber*



Open Access Article. Published on 03 December 2025. Downloaded on 2/27/2026 8:14:31 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

PAPERS

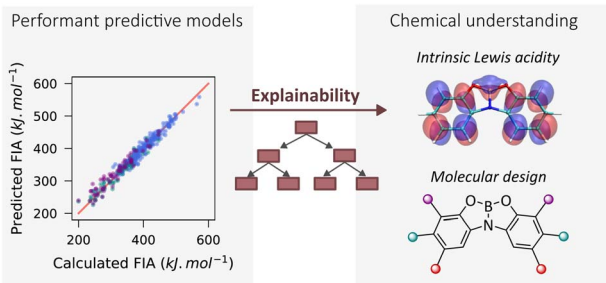
3610



Unsupervised multi-clustering and decision-making strategies for 4D-STEM orientation mapping

Junhao Cao, Nicolas Folastre, Gozde Oney, Edgar Rauch, Stavros Nicolopoulos, Partha Pratim Das and Arnaud Demortière*

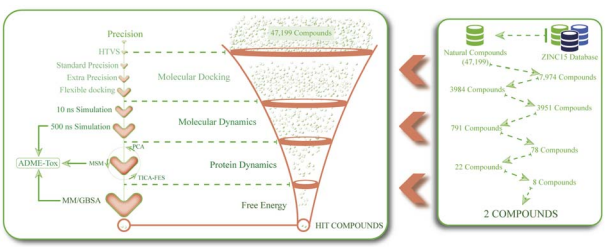
3623



Constructing and explaining machine learning models for the exploration and design of boron-based Lewis acids

Juliette Fenogli,* Laurence Grimaud* and Rodolphe Vuilleumier*

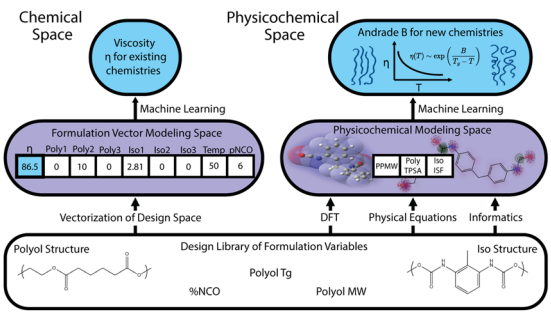
3635



Database mining of ZINC15 natural compounds reveals potential thyroid receptor β agonists for NAFLD management: an *in silico* study

Ahmet Buğra Ortaakarsu,* Michel Hosny, Mansour Sobeh and Mohamed A. O. Abdelfattah

3652



Machine learning of polyurethane prepolymer viscosity: a comparison of chemical and physicochemical approaches

Joseph A. Pugar, Calvin Gang, Isabelle Millan, Karl Haider and Newell R. Washburn*

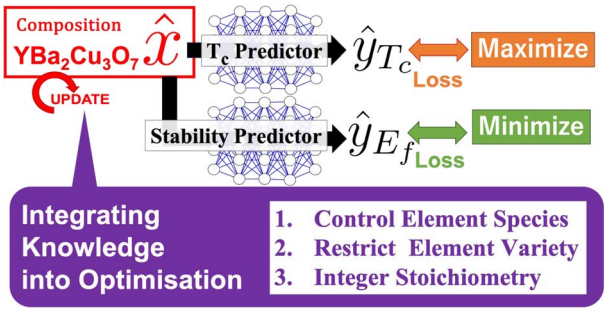
This journal is © The Royal Society of Chemistry 2025

Open Access Article. Published on 03 December 2025. Downloaded on 2/27/2026 8:14:31 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

3662

A straightforward gradient-based approach for designing superconductors with high critical temperature: exploiting domain knowledge *via* adaptive constraints

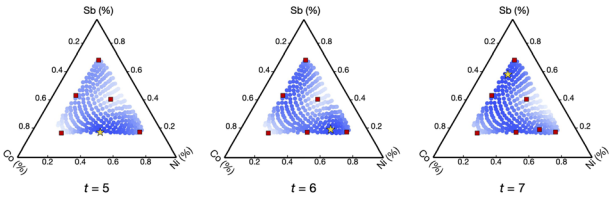
Akihiro Fujii,* Anh Khoa Augustin Lu, Koji Shimizu and Satoshi Watanabe



3674

Active learning path-dependent properties using a cloud-based materials acceleration platform

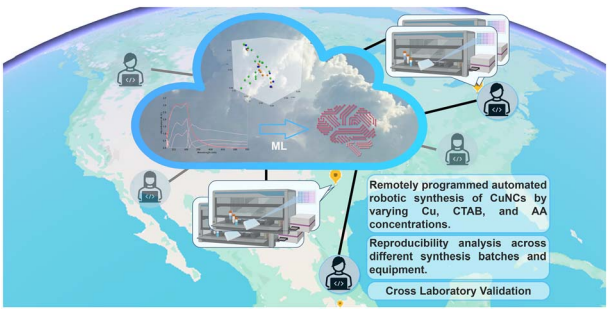
Dan Guevarra, Michael J. Statt,* Kostiantyn Popovich, Brian A. Rohr,* John M. Gregoire, Kevin Tran, Santosh K. Suram, Joel A. Haber* and Willie Neiswanger*



3683

Cross-laboratory validation of machine learning models for copper nanocluster synthesis using cloud-based automated platforms

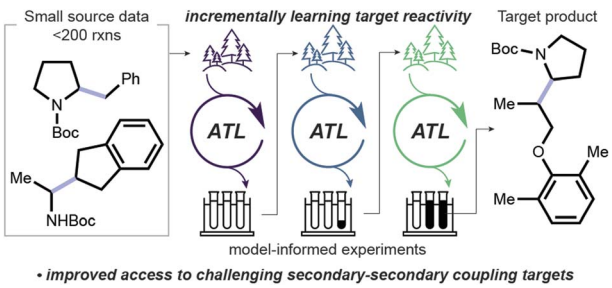
Ricardo Montoya-Gonzalez, Rosa de Guadalupe González-Huerta, Martha Leticia Hernández-Pichardo and Subha R. Das*



3693

Prospective active transfer learning on the formal coupling of amines and carboxylic acids to form secondary alkyl bonds

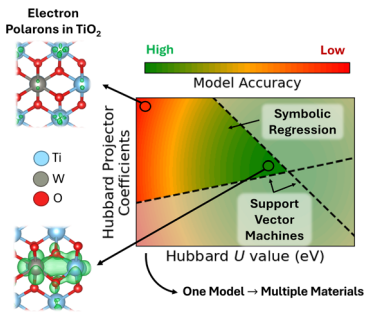
Eunjae Shim, Ambuj Tewari, Paul M. Zimmerman* and Tim Cernak*



Open Access Article. Published on 03 December 2025. Downloaded on 2/27/2026 8:14:31 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

PAPERS

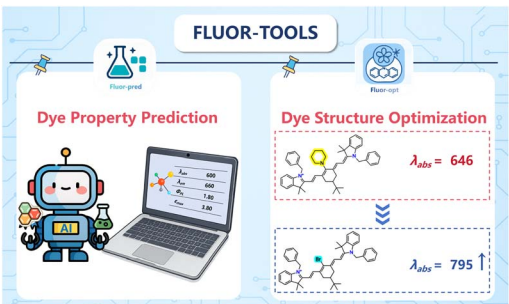
3701



Machine learning generalised DFT+*U* projectors in a numerical atom-centred orbital framework

Amit Chaudhari, Kushagra Agrawal and Andrew J. Logsdail*

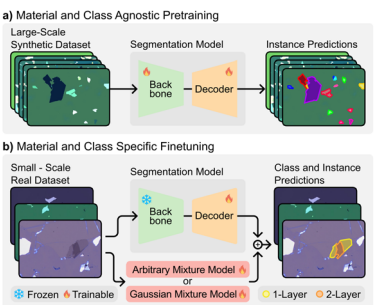
3728



Fluor-tools: an integrated platform for dye property prediction and structure optimization

Wenxiang Song, Yuyang Zhang, Le Xiong, Xinmin Li, Jingwei Zhang, Guixia Liu, Weihua Li, Youjun Yang* and Yun Tang*

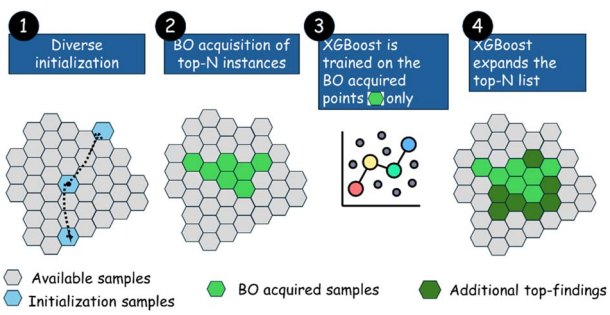
3744



MaskTerial: a foundation model for automated 2D material flake detection

Jan-Lucas Uslu,* Alexey Nekrasov, Alexander Hermans, Bernd Beschoten, Bastian Leibe, Lutz Waldecker and Christoph Stampfer

3753



Navigating materials design spaces with efficient Bayesian optimization: a case study in functionalized nanoporous materials

Panagiotis Krokidas,* Vassilis Gkatsis, John Theocharis and George Giannakopoulos

This journal is © The Royal Society of Chemistry 2025

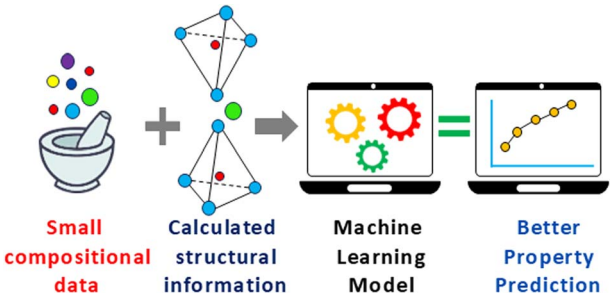
Open Access Article. Published on 03 December 2025. Downloaded on 2/27/2026 8:14:31 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

PAPERS

3764

An improved machine learning strategy using structural features to predict the glass transition temperature of oxide glasses

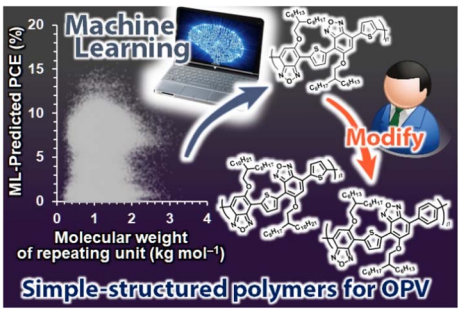
Satwinder Singh Danewalia* and Kulvir Singh



3774

Design of simple-structured conjugated polymers for organic solar cells by machine learning-assisted structural modification and experimental validation

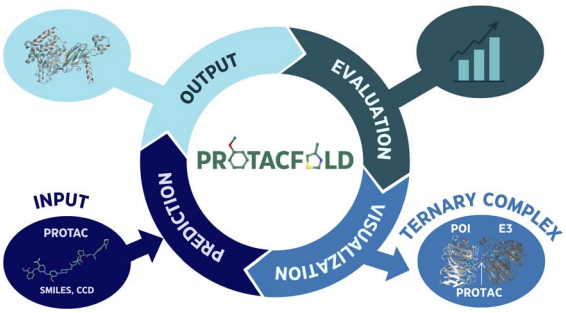
Shogo Tadokoro, Ryosuke Kamimura, Fumitaka Ishiwari and Akinori Saeki*



3782

Predicting PROTAC-mediated ternary complexes with AlphaFold3 and Boltz-1

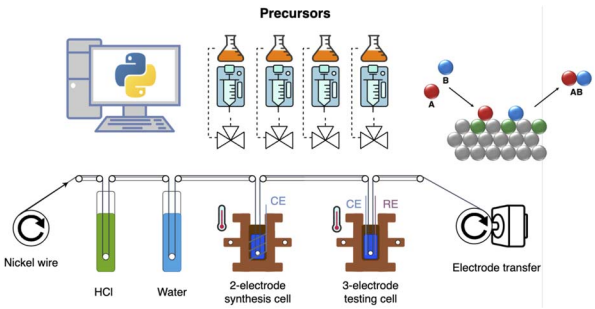
Nils Dunlop, Francisco Erazo, Farzaneh Jalalypour and Rocío Mercado*



3810

CatBot – a high-throughput catalyst synthesis and testing system with roll to roll transfer

Paolo Vincenzo Freiesleben de Blasio,* Rune Kruger, Nis Fisker-Bødker, Jin Hyun Chang and Christodoulos Chatzichristodoulou



Open Access Article. Published on 03 December 2025. Downloaded on 2/27/2026 8:14:31 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

PAPERS

3818

Multi-modal contrastive learning for chemical structure elucidation with VibraCLIP

Pau Rocabert-Oriols, Camilla Lo Conte, Núria López and Javier Heras-Domingo*

CORRECTION

3828

Correction: Beyond training data: how elemental features enhance ML-based formation energy predictions

Hamed Mahdavi,* Vasant Honavar and Dane Morgan

This journal is © The Royal Society of Chemistry 2025