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IN THIS ISSUE

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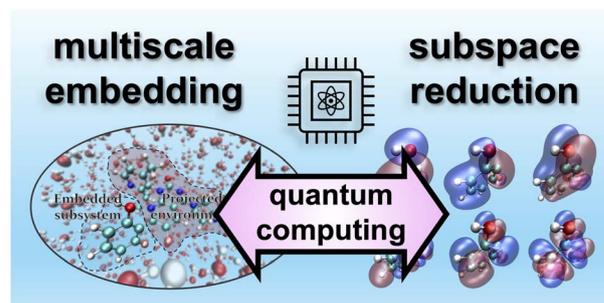
Inside cover
See Ge Lei and Samuel J. Cooper, pp. 3455–3465. Image reproduced by permission of Ge Lei and Samuel J. Cooper from *Digital Discovery*, 2025, 4, 3455. Image created with the use of Google Gemini and Adobe Photoshop Generative Fill.

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*

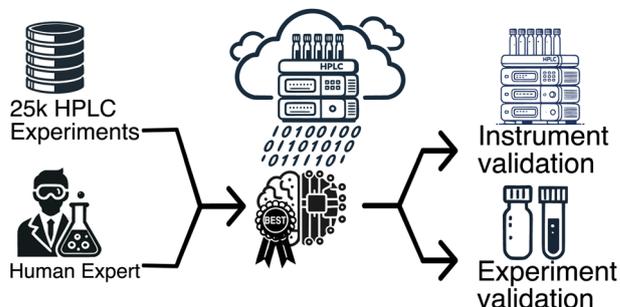


PAPERS

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*



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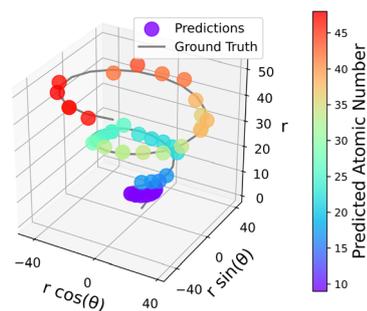


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3455

Do Llamas understand the periodic table?

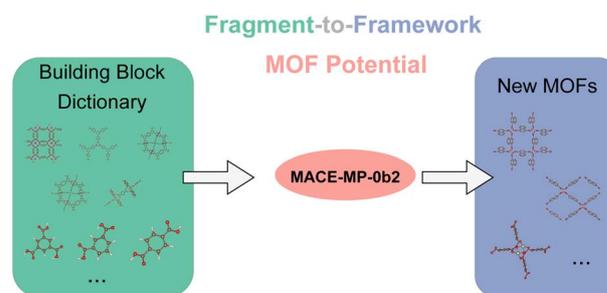
Ge Lei* and Samuel J. Cooper



3466

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

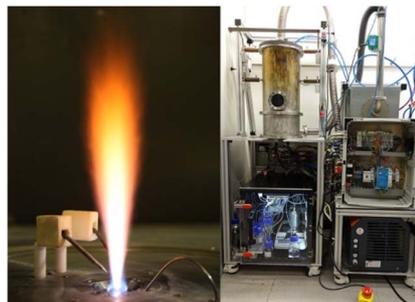
Xiaoqi Zhang, Yutao Li, Xin Jin and Berend Smit*



3478

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

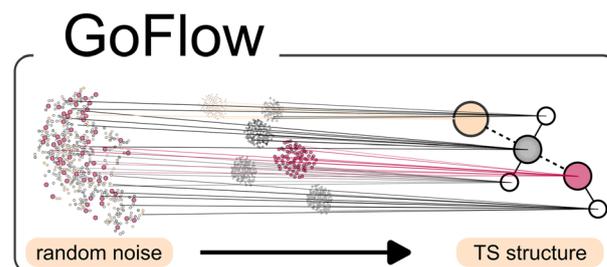
Konstantin M. Engel, Patrik O. Willi, Robert N. Grass and Wendelin J. Stark*



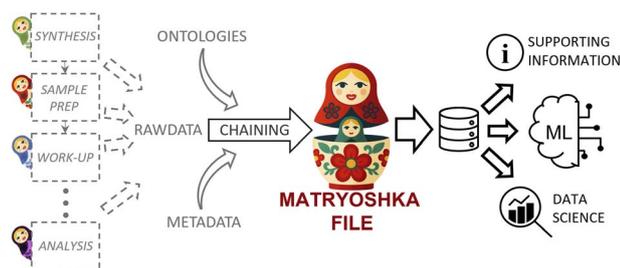
3492

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*



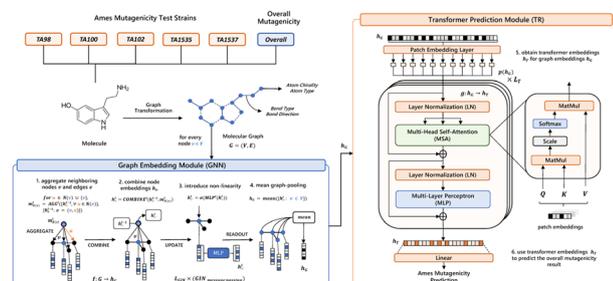
3502



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 Grognez

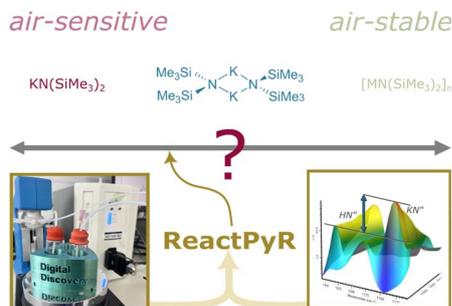
3515



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

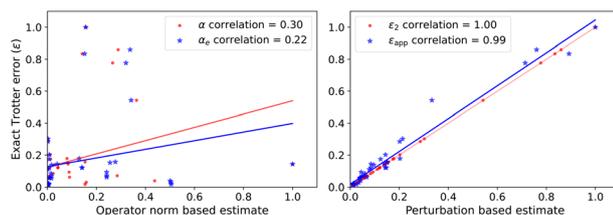
3533



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

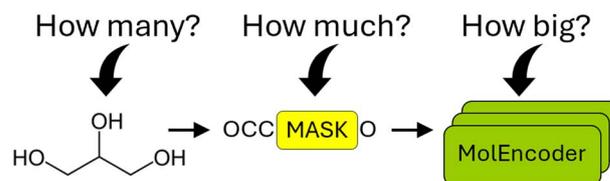
Shashank G. Mehendale, Luis A. Martínez-Martínez, Pratham Divakar Kamath and Artur F. Izmaylov*



3552

MolEncoder: towards optimal masked language modeling for molecules

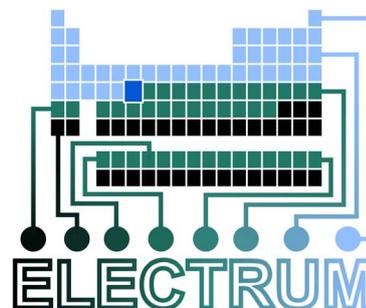
Fabian P. Krüger,* Nicklas Österbacka, Mikhail Kabeshov, Ola Engkvist and Igor Tetko



3567

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

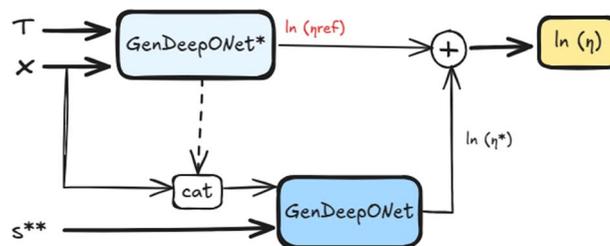
Markus Orsi* and Angelo Frei*



3578

Generalized DeepONets for viscosity prediction using learned entropy scaling references

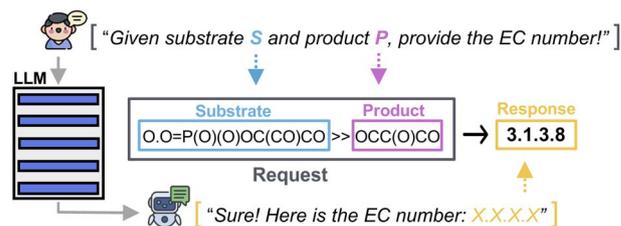
Maximilian Fleck,* Marcelle B. M. Spera, Samir Darouich, Timo Klenk and Niels Hansen*



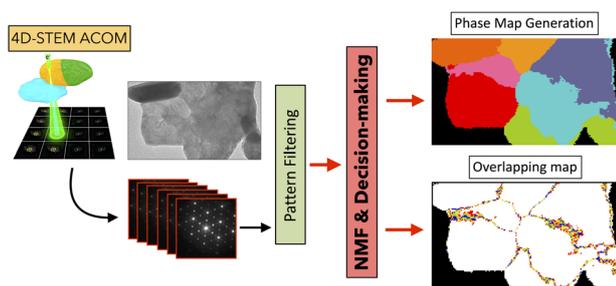
3588

Leveraging large language models for enzymatic reaction prediction and characterization

Lorenzo Di Fruscia and Jana M. Weber*



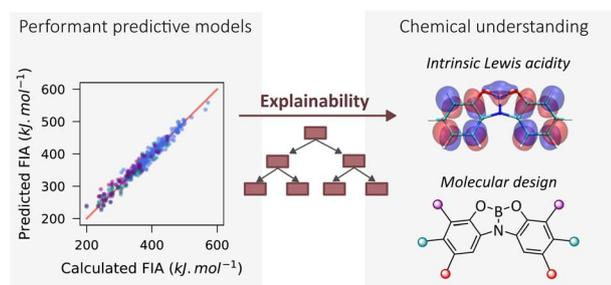
3610



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*

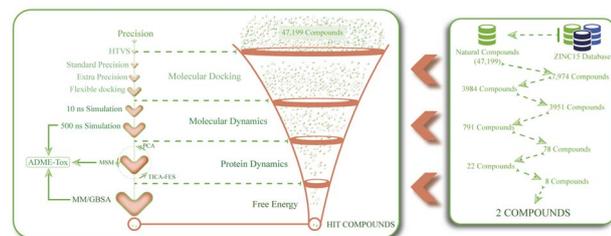
3623



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

Juliette Fenogli,* Laurence Grimaud* and Rodolphe Vuilleumier*

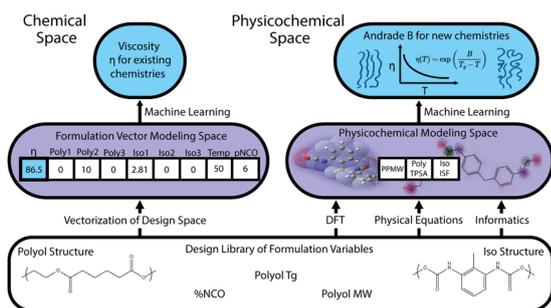
3635



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

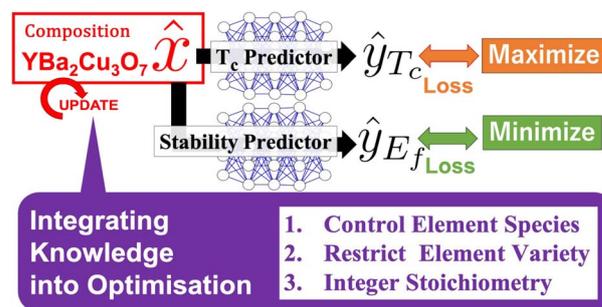
Joseph A. Pugar, Calvin Gang, Isabelle Millan, Karl Haider and Newell R. Washburn*



3662

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

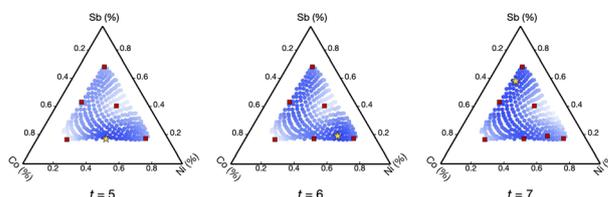
Akihiro Fujii,* Anh Khoa Augustin Lu, Koji Shimizu and Satoshi Watanabe



3674

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

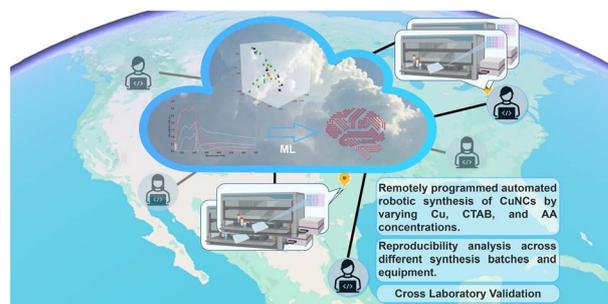
Dan Guevarra, Michael J. Statt,* Kostyantyn Popovich, Brian A. Rohr,* John M. Gregoire, Kevin Tran, Santosh K. Suram, Joel A. Haber* and Willie Neiswanger*



3683

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

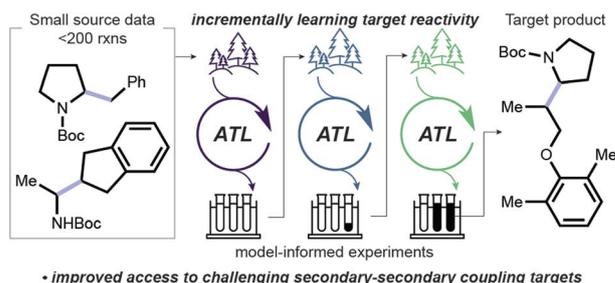
Ricardo Montoya-Gonzalez, Rosa de Guadalupe González-Huerta, Martha Leticia Hernández-Pichardo and Subha R. Das*



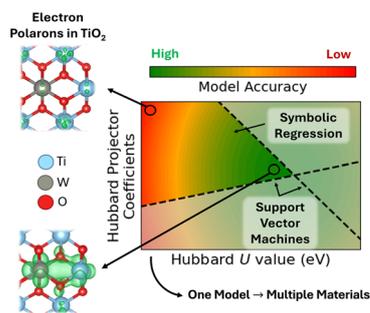
3693

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*



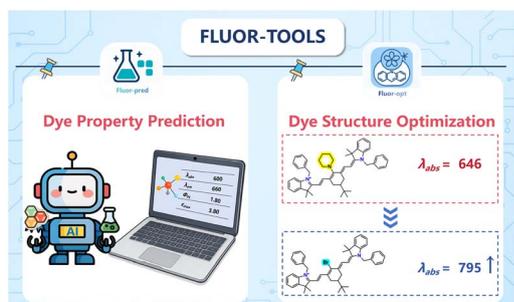
3701



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

Amit Chaudhari, Kushagra Agrawal and Andrew J. Logsdail*

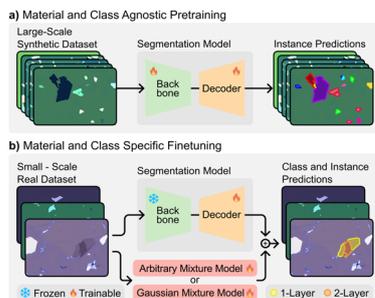
3728



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*

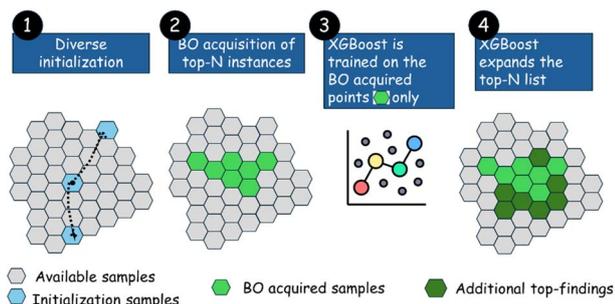
3744



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

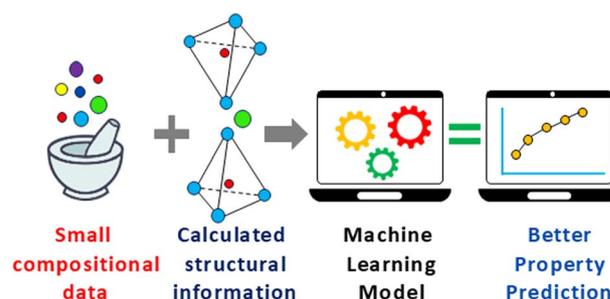
Panagiotis Krokidas,* Vassilis Gkatsis, John Theocharis and George Giannakopoulos



3764

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

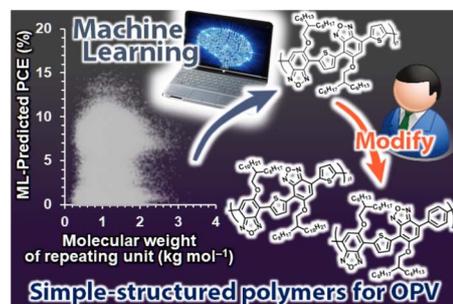
Satwinder Singh Danewalia* and Kulvir Singh



3774

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

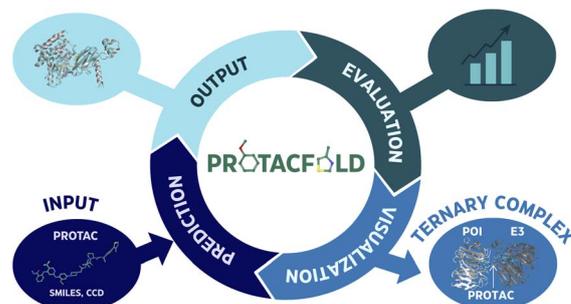
Shogo Tadokoro, Ryosuke Kamimura, Fumitaka Ishiwari and Akinori Saeki*



3782

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

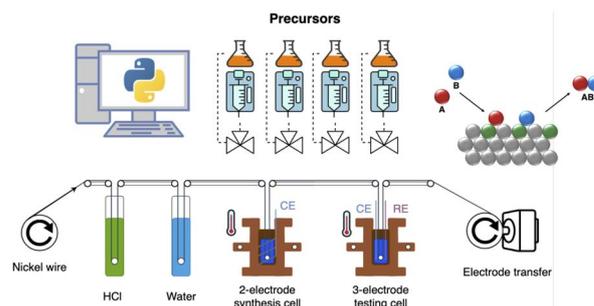
Nils Dunlop, Francisco Erazo, Farzaneh Jalalypour and Rocío Mercado*



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



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

