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(8) 1977–2274 (2025)

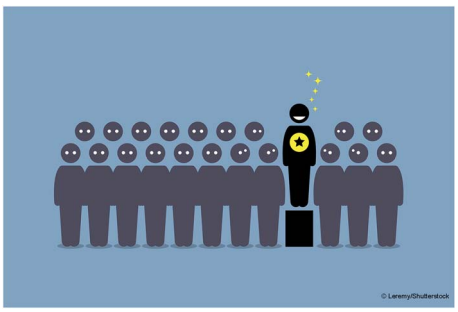
Cover
See Jan Gerit Brandenburg *et al.*, pp. 1991–2000. Image reproduced by permission of Merck KGaA, Darmstadt, Germany from *Digital Discovery*, 2025, **4**, 1991.

Inside cover
See Maciej Haranczyk *et al.*, pp. 2001–2011. Image reproduced by permission of Alex Mascaraque León from *Digital Discovery*, 2025, **4**, 2001. Created with the use of Google's Gemini model *via* Google Cloud Platform.

EDITORIAL

1987

Outstanding Reviewers for *Digital Discovery* in 2024

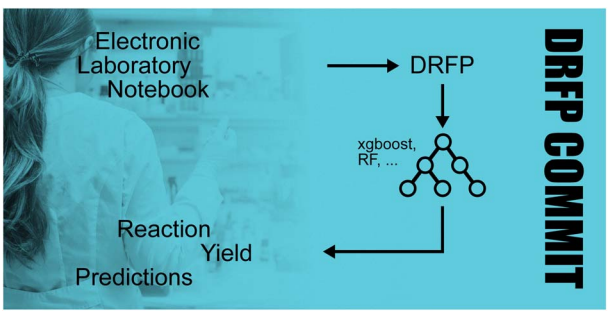


COMMIT

1988

Commit: Reaction classification and yield prediction using the differential reaction fingerprint DRFP

Daniel Probst



Industrial Chemistry & Materials

GOLD OPEN ACCESS

Focus on industrial chemistry
Advance material innovations
Highlight interdisciplinary feature

Innovative.
Interdisciplinary.
Problem solving

APCs currently waived

Learn more about ICM
Submit your high-quality article

@IndChemMater

@IndChemMater

rsc.li/icm

ROYAL SOCIETY OF CHEMISTRY

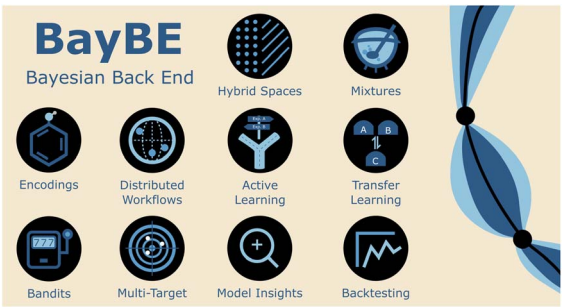
Industrial Chemistry & Materials

PAPERS

1991

BayBE: a Bayesian Back End for experimental planning in the low-to-no-data regime

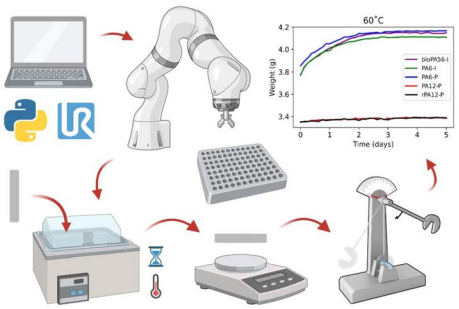
Martin Fitzner, Adrian Šošić, Alexander V. Hopp, Marcel Müller, Rim Rihana, Karin Hrovatin, Fabian Liebig, Mathias Winkel, Wolfgang Halter and Jan Gerit Brandenburg*



2001

Streamlining material degradation testing: collaborative robotics for specimen monitoring

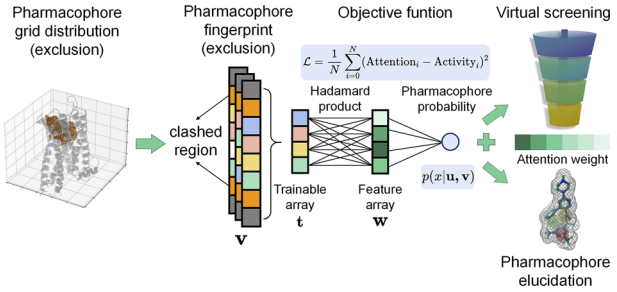
Brody Stack, Miguel Hernández-del-Valle, Alex Mascaraque-León, Petronela Chovancová, Loris Langeois, Jacob Porath, Juan P. Fernandez-Blazquez, Mónica Echeverry-Rendón and Maciej Haranczyk*



2012

Enhancing multifunctional drug screening *via* artificial intelligence

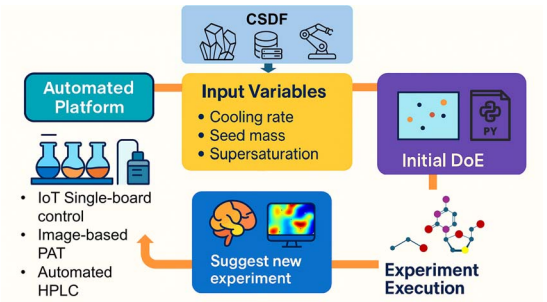
Junlin Dong,* Chenyang Wu,* Tianle Lu,* Shiyu Wang,* Wenjin Zhan, Marc Xu, Bing Wang, Zhenquan Hu, Horst Vogel and Shuguang Yuan



2025

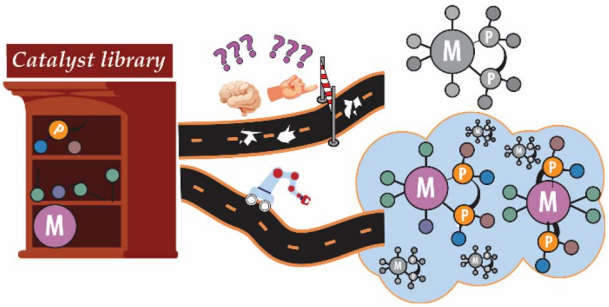
Automated scale-up crystallisation DataFactory for model-based pharmaceutical process development: a Bayesian case study

Thomas Pickles, Youcef Leghrib, Matt Weisshaar, Mikhail Goncharuk, Peter Timperman, Timothy Doherty, David D. Ford, Jonathan Moores, Alastair J. Florence and Cameron J. Brown*



PAPERS

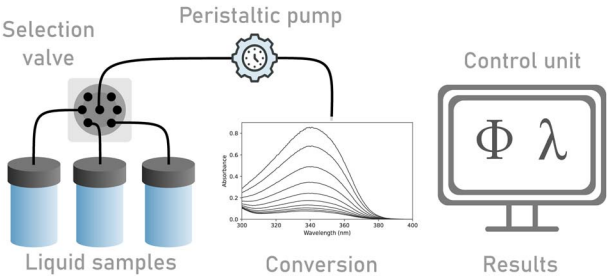
2033



Unveiling the impact of ligand configurations and structural fluxionality on virtual screening of transition-metal complexes

Adarsh V. Kalikadien, Niels J. van der Lem, Cecile Valsecchi, Laurent Lefort and Evgeny A. Pidko*

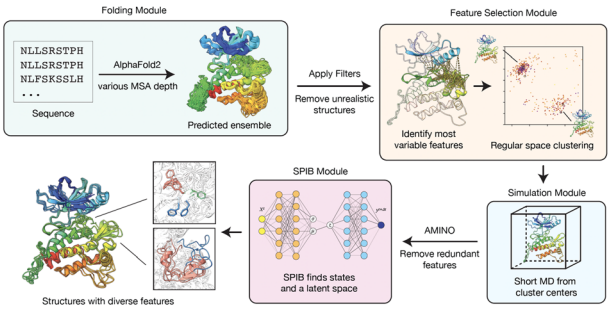
2045



An automated photo-isomerisation and kinetics characterisation system for molecular photoswitches

Jacob Lynge Elholm, Paulius Baronas, Paul A. Gueben, Victoria Gneiting, Helen Hölzel and Kasper Moth-Poulsen*

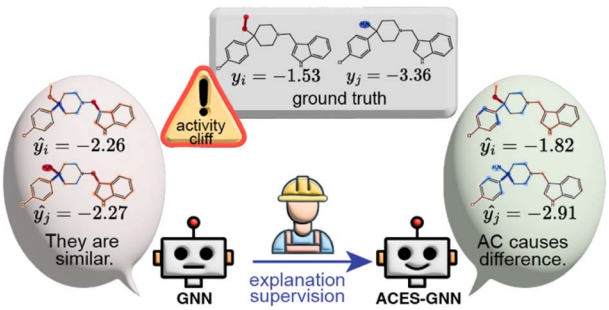
2052



af2rave: protein ensemble generation with physics-based sampling

Da Teng, Vanessa J. Meraz, Akashnathan Aranganathan, Xinyu Gu and Pratyush Tiwary*

2062



ACES-GNN: can graph neural network learn to explain activity cliffs?

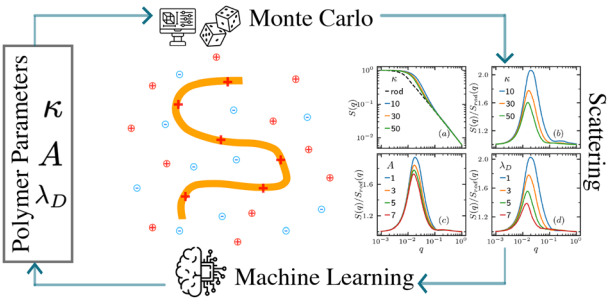
Xu Chen, Dazhou Yu, Liang Zhao and Fang Liu*

PAPERS

2075

Machine learning inversion from small-angle scattering for charged polymers

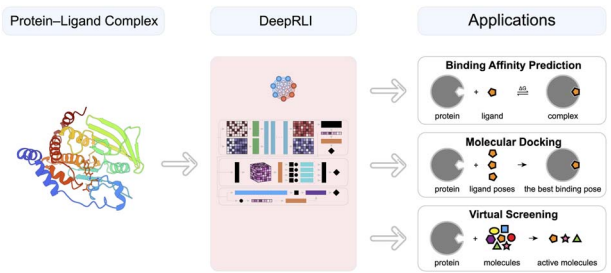
Lijie Ding, Chi-Huan Tung, Jan-Michael Y. Carrillo, Wei-Ren Chen and Changwoo Do*



2083

DeepRLI: a multi-objective framework for universal protein–ligand interaction prediction

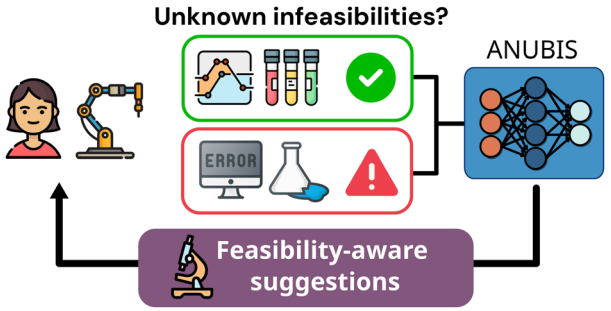
Haoyu Lin, Jintao Zhu, Shiwei Wang, Yibo Li, Jianfeng Pei* and Luhua Lai*



2104

Anubis: Bayesian optimization with unknown feasibility constraints for scientific experimentation

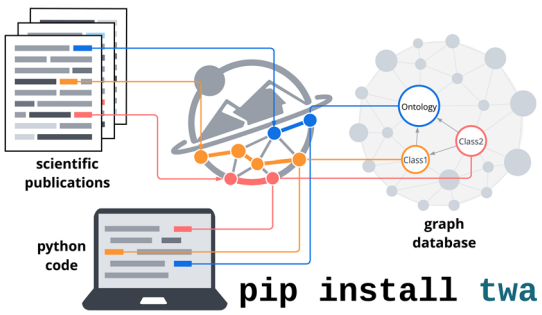
Riley J. Hickman,* Gary Tom, Yunheng Zou, Matteo Aldeghi and Alán Aspuru-Guzik*



2123

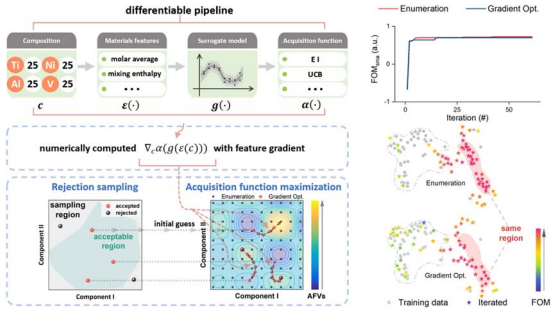
twa: The World Avatar Python package for dynamic knowledge graphs and its application in reticular chemistry

Jiaru Bai, Simon D. Rihm, Aleksandar Kondinski, Fabio Saluz, Xinhong Deng, George Brownbridge, Sebastian Mosbach, Jethro Akroyd and Markus Kraft*



PAPERS

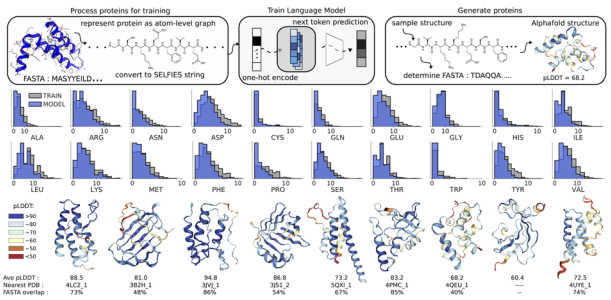
2136



Leveraging feature gradient for efficient acquisition function maximization in material composition design

Yuehui Xian, Yunfan Wang, Pengfei Dang, Xinquan Wan, Yumei Zhou,* Xiangdong Ding,* Jun Sun and Dezhen Xue*

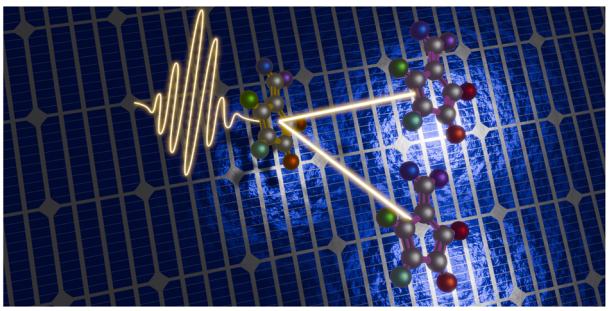
2150



Chemical language models can generate biomolecules atom-by-atom

Kevin Zhu, Daniel Flam-Shepherd and Alán Aspuru-Guzik*

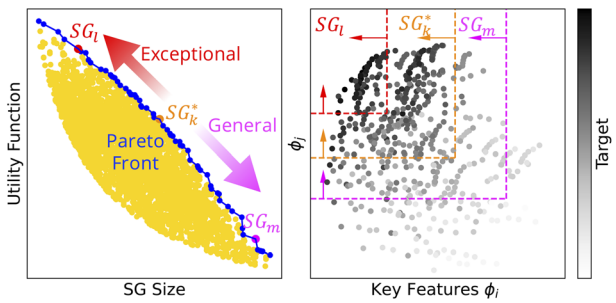
2156



Pursuit of singlet fission fulvene candidates using inverse design

Irene Casademont-Reig,* Roger Monreal-Corona, Eline Desmedt, Freija De Vleeschouwer* and Mercedes Alonso*

2175



Coherent collections of rules describing exceptional materials identified with a multi-objective optimization of subgroups

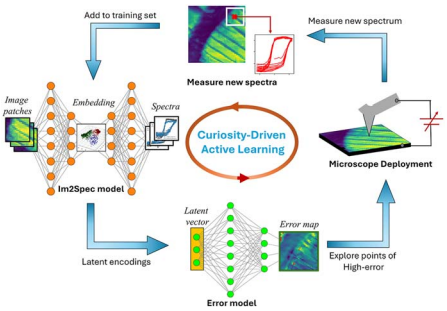
Lucas Foppa* and Matthias Scheffler

PAPERS

2188

Curiosity driven exploration to optimize structure–property learning in microscopy

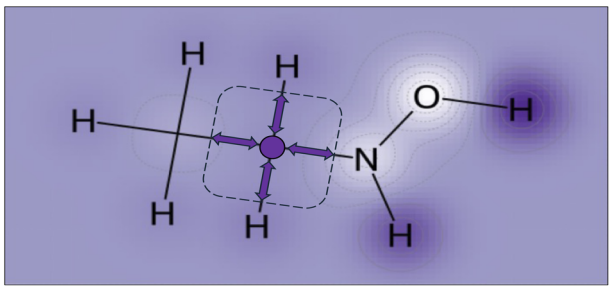
Aditya Vatsavai, Ganesh Narasimha, Yongtao Liu, Jawad Chowdhury, Jan-Chi Yang, Hiroshi Funakubo, Maxim Ziatdinov and Rama Vasudevan*



2198

PIL-Net: a physics-informed graph convolutional network for predicting atomic multipoles

Caitlin Whitter,* Alex Pothen and Aurora Clark

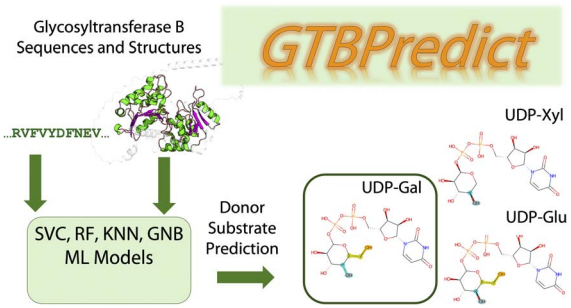


Depiction of the atomic charge distribution of C_2H_7NO with a graph convolution around a Carbon atom.

2214

Decoding substrate specificity determining factors in glycosyltransferase-B enzymes – insights from machine learning models

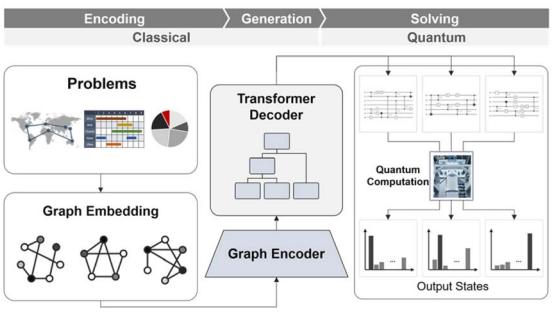
Samantha G. Hennen, Yannick J. Bomble, Breanna R. Urbanowicz and Vivek S. Bharadwaj*



2229

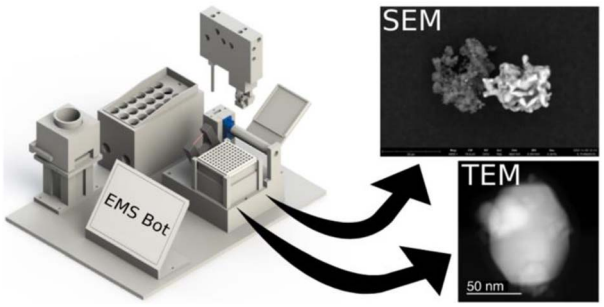
Generative quantum combinatorial optimization by means of a novel conditional generative quantum eigensolver

Shunya Minami,* Kouhei Nakaji, Yohichi Suzuki, Alán Aspuru-Guzik and Tadashi Kadowaki



PAPERS

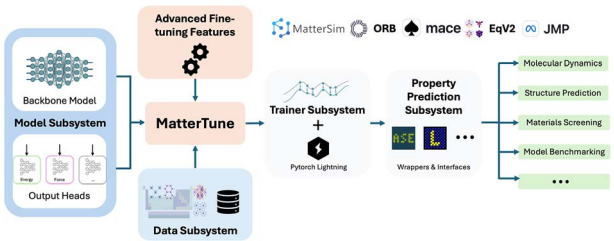
2244



Automated electron microscopy sample preparation system

David Milsted, Tara P. Mishra, Lauren N. Walters, Yuxing Fei, Bernardus Rendy, Pragnay Nevatia, Haegyeom Kim and Gerbrand Ceder*

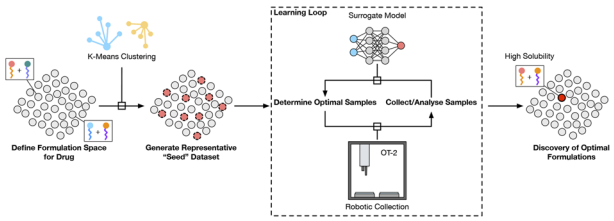
2253



MatterTune: an integrated, user-friendly platform for fine-tuning atomistic foundation models to accelerate materials simulation and discovery

Lingyu Kong, Nima Shoghi, Guoxiang Hu, Pan Li and Victor Fung*

2263



Efficient discovery of new medicine formulations using a semi-self-driven robotic formulator

Helena Ros, Youssef Abdalla, Michael T. Cook* and David Shorthouse*