

## IN THIS ISSUE

ISSN 2635-098X CODEN DDIAI 4(11) 3055–3414 (2025)



**Cover**  
See Fanjin Wang *et al.*, pp. 3066–3077. Image reproduced by permission of Fanjin Wang from *Digital Discovery*, 2025, 4, 3066.



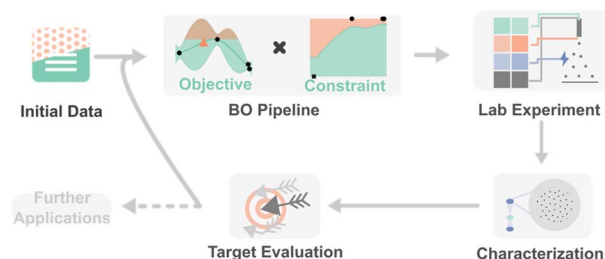
**Inside cover**  
See Jason Hattrick-Simpers *et al.*, pp. 3078–3091. Image reproduced by permission of Seyed Shayan Mousavi Masouleh from *Digital Discovery*, 2025, 4, 3078.

## PAPERS

3066

### Constrained composite Bayesian optimization for rational synthesis of polymeric particles

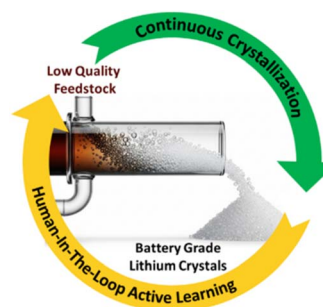
Fanjin Wang,\* Maryam Parhizkar, Anthony Harker and Mohan Edirisinghe



3078

### Human-AI synergy in adaptive active learning for continuous lithium carbonate crystallization optimization

Shayan Mousavi Masouleh, Corey A. Sanz, Ryan P. Jansonius, Cara Cronin, Jason E. Hein and Jason Hattrick-Simpers\*



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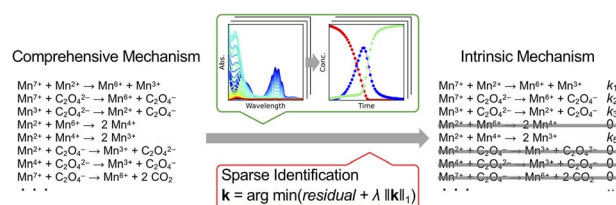
[rsc.li/EESCatalysis](https://rsc.li/EESCatalysis)

Fundamental questions  
Elemental answers

3092

## Sparse identification of chemical reaction mechanisms from limited concentration profiles

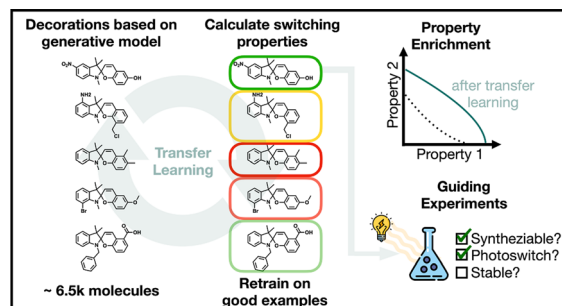
Shun Hayashi\*



3098

## Machine learning driven design of spirocyan photoswitches

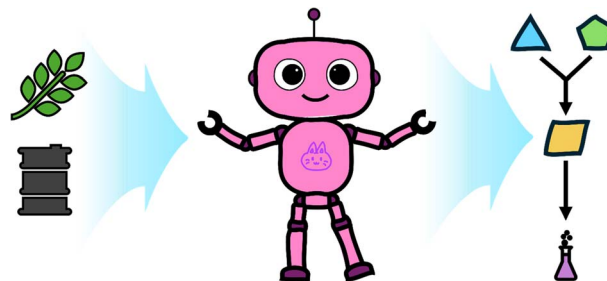
Robert Strothmann, Mehran Amanpur, Tomáš Neveselý, Stefan Hecht,\* Karsten Reuter\* and Johannes T. Margraf\*



3109

## Discovery of hybrid chemical synthesis pathways with DORAnet

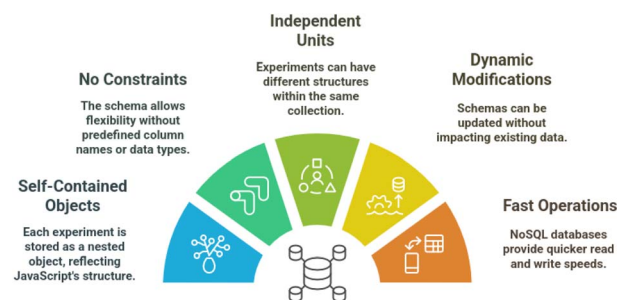
Quan Zhang, William W. Sprague, Shivani S. Kozarekar, Stefan C. Pate, Taylor Uekert and Linda J. Broadbelt\*



3126

## SEARS: a lightweight FAIR platform for multi-lab materials experiments and closed-loop optimization

Ronak Tali, Ankush Kumar Mishra, Devesh Lohia, Jacob Paul Mauthe, Justin Scott Neu, Sung-Joo Kwon, Yusuf Olanrewaju, Aditya Balu, Goce Trajcevski, Franky So, Wei You, Aram Amassian\* and Baskar Ganapathysubramanian\*



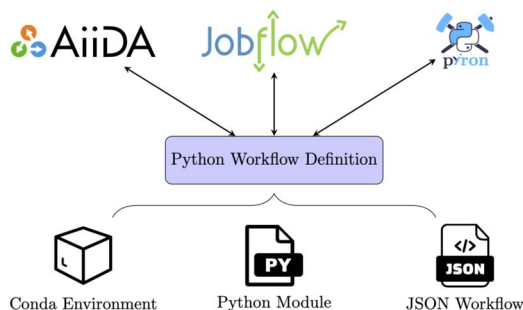
3137



### MARCUS: molecular annotation and recognition for curating unravalled structures

Kohulan Rajan, Viktor Weißenborn, Laurin Lederer, Achim Zielesny and Christoph Steinbeck\*

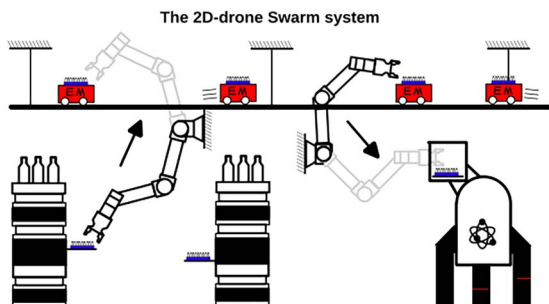
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### A python workflow definition for computational materials design

Jan Janssen,\* Janine George, Julian Geiger, Marnik Berx, Xing Wang, Christina Ertural, Jörg Schaarschmidt, Alex M. Ganose, Giovanni Pizzi, Tilmann Hickel and Jörg Neugebauer

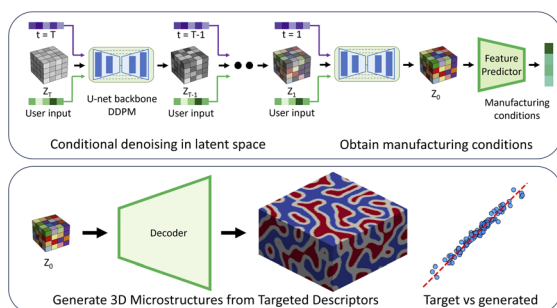
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### The 2D-drone swarm, a safe open-source sample transfer system for fully automated laboratories

Edy Mariano,\* Yannis Coderey, Yasmine El Goumi, Jasper Tan, Tanguy Cavagna, Jean-Charles Cousty, Vincenzo Scamarcio, Josie Hughes and Pascal Miéville

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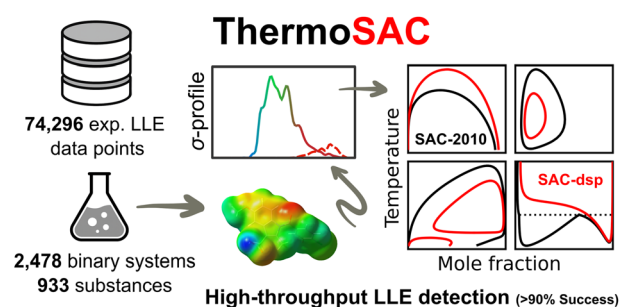
### 3D multiphase heterogeneous microstructure generation using conditional latent diffusion models

Nirmal Baishnab, Ethan Herron, Aditya Balu, Soumik Sarkar, Adarsh Krishnamurthy\* and Baskar Ganapathysubramanian\*



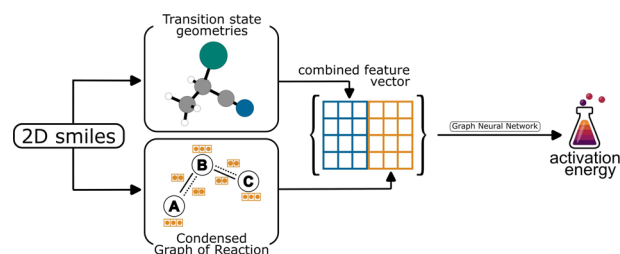
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## High-throughput application and evaluation of the COSMO-SAC model for predictions of liquid–liquid equilibria

Ivan Antolović, Simon Stephan and Jadran Vrabc\*<sup>\*</sup>

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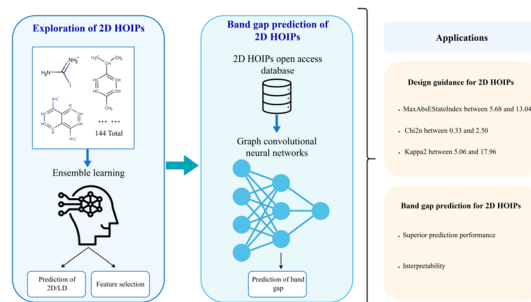
## Graph-based prediction of reaction barrier heights with on-the-fly prediction of transition states

Johannes Karwounopoulos, Jasper De Landsheere, Leonard Galustian, Tobias Jechtl and Esther Heid\*<sup>\*</sup>

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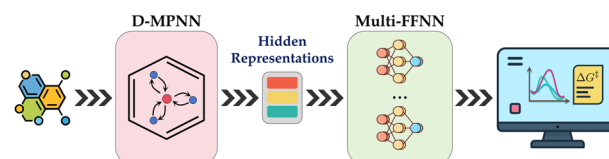
## Design guidance and band gap prediction of two-dimensional hybrid organic–inorganic perovskites by ensemble learning and graph convolutional neural networks

Jianfei Liu, Xia Cai,\* Lin Wang and Yiqiang Zhan

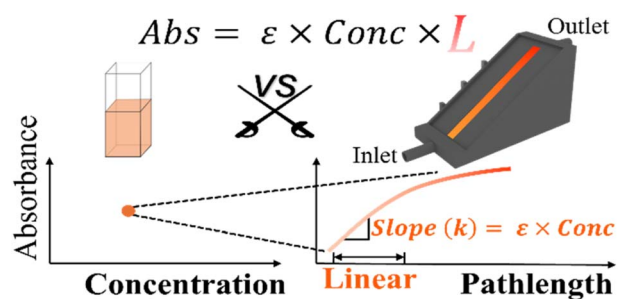


3227

## Harnessing surrogate models for data-efficient predictive chemistry: descriptors vs. learned hidden representations

Guanming Chen and Thijs Stuyver\*<sup>\*</sup>

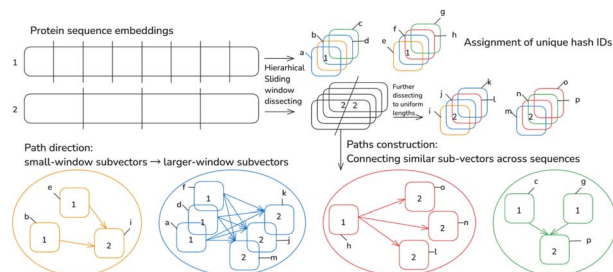
3238



### Variable pathlength cell for internal data validation in computer vision

Xiangyu Liu, Namita Sharma, Aldrik H. Velders and Vittorio Saggiomo\*

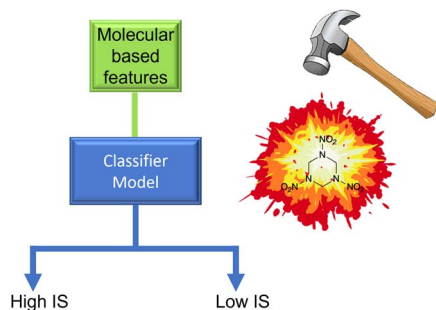
3245



### MAAPE: a tool for modular evolution analysis of protein embeddings

Xiaoyu Wang, Qiandi Gao, Heqian Zhang, Jiaquan Huang and Zhiwei Qin\*

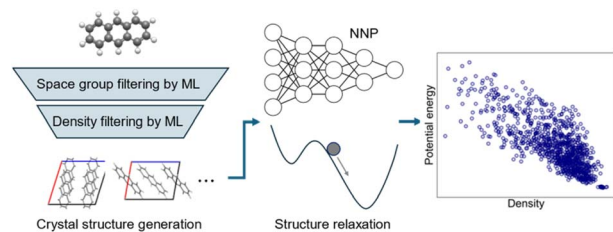
3260



### Understanding impact sensitivity of energetic molecules by supervised machine learning

Heather M. Quayle, Karthik Mohan, Sohan Seth, Colin R. Pulham and Carole A. Morrison\*

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### Crystal structure prediction of organic molecules by machine learning-based lattice sampling and structure relaxation

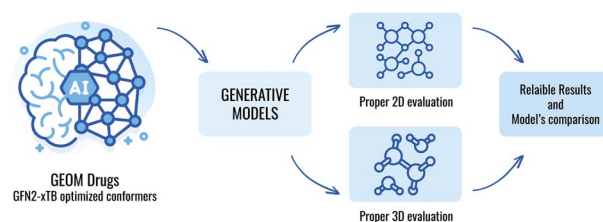
Takuya Taniguchi\* and Ryo Fukasawa



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## GEOM-drugs revisited: toward more chemically accurate benchmarks for 3D molecule generation

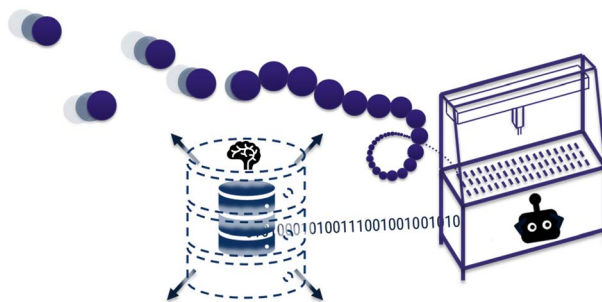
Filipp Nikitin, Ian Dunn, David Ryan Koes and Olexandr Isayev\*



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## Unveiling the knowledge of a RAFT polymerization database obtained from an automated parallel synthesizer

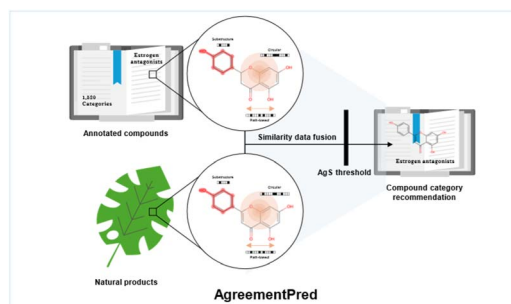
Michael Ringleb, Yannik Köster, Stefan Zechel and Ulrich S. Schubert\*



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## AgreementPred: a cheminformatic framework for drug and natural product category recommendation based on multi-representation structural similarity data fusion

Chayanis Sutcharitchan, Boyang Wang, Dingfan Zhang, Qingyuan Liu, Tingyu Zhang, Peng Zhang and Shao Li\*



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## Optimal message passing for molecular prediction is simple, attentive and spatial

Alma C. Castañeda-Leautaud\* and Rommie E. Amaro\*



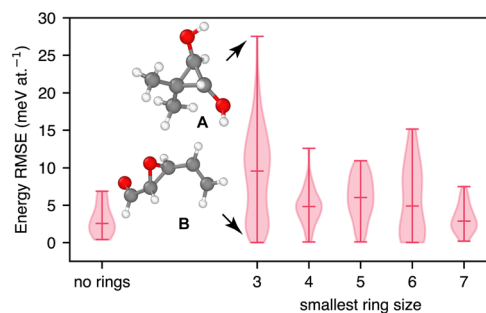


## PAPERS

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### Assessing zero-shot generalisation behaviour in graph-neural-network interatomic potentials

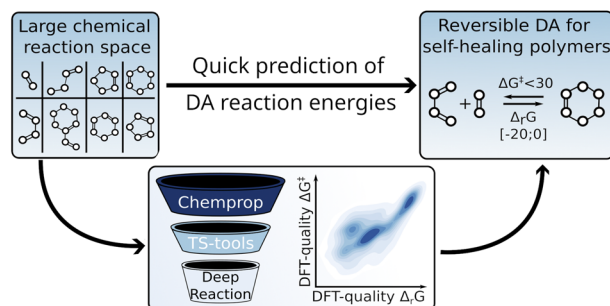
Chiheb Ben Mahmoud,\* Zakariya El-Machachi, Krystian A. Gierczak, John L. A. Gardner and Volker L. Deringer



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### Screening Diels–Alder reaction space to identify candidate reactions for self-healing polymer applications

Maxime Ferrer,\* Bowen Deng, Javier E. Alfonso-Ramos and Thijs Stuyver\*



## CORRECTION

3411

### Correction: 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\*

