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



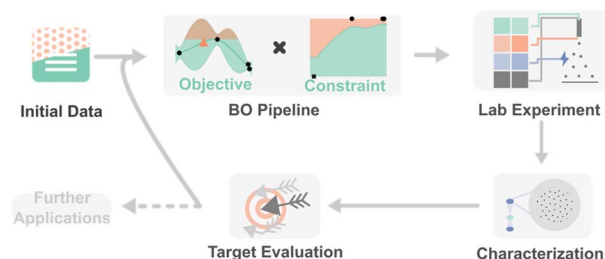
Inside cover
See Jason Hattrick-Simpers *et al.*, pp. 3078–3091. Image reproduced by permission of Seyed Shayan Mousavi Masouleh from *Digital Discovery*, 2025, 4, 3078.

PAPERS

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Constrained composite Bayesian optimization for rational synthesis of polymeric particles

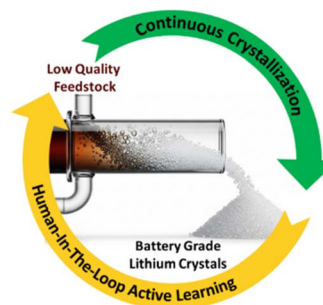
Fanjin Wang,* Maryam Parhizkar, Anthony Harker and Mohan Edirisinghe



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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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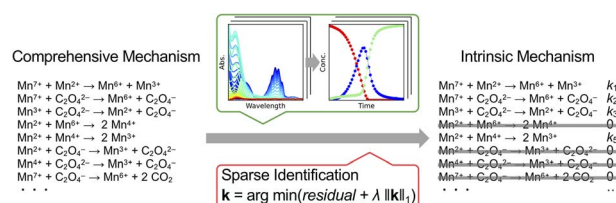
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Fundamental questions
Elemental answers

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Sparse identification of chemical reaction mechanisms from limited concentration profiles

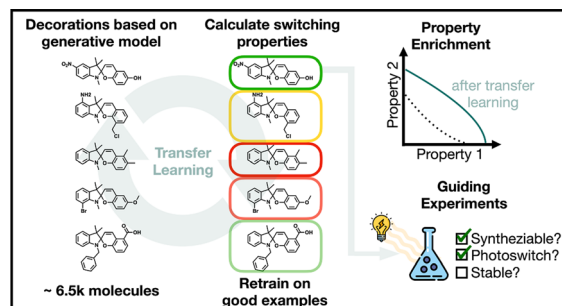
Shun Hayashi*



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Machine learning driven design of spiropyran photoswitches

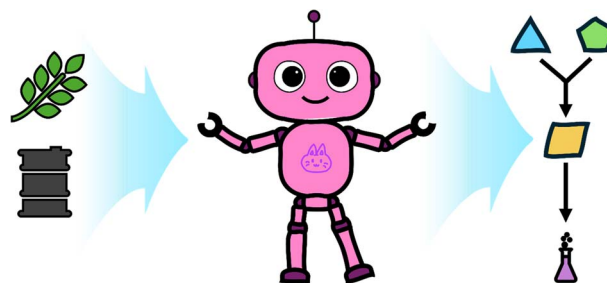
Robert Strothmann, Mehran Amanpur, Tomáš Neveselý, Stefan Hecht,* Karsten Reuter* and Johannes T. Margraf*



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Discovery of hybrid chemical synthesis pathways with DORAnet

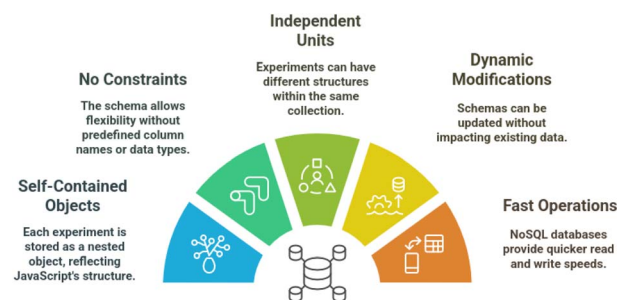
Quan Zhang, William W. Sprague, Shivani S. Kozarekar, Stefan C. Pate, Taylor Uekert and Linda J. Broadbelt*



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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*



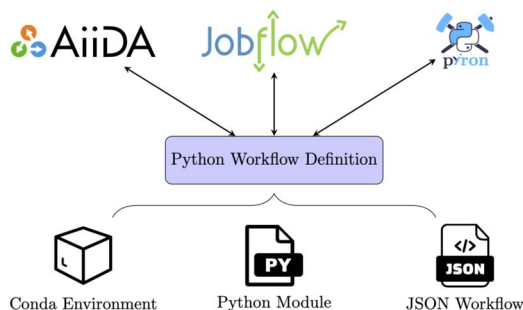
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MARCUS: molecular annotation and recognition for curating unravalled structures

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

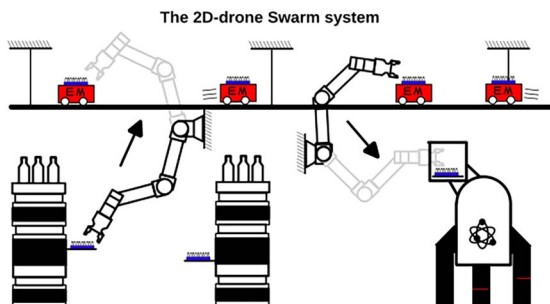
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A python workflow definition for computational materials design

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

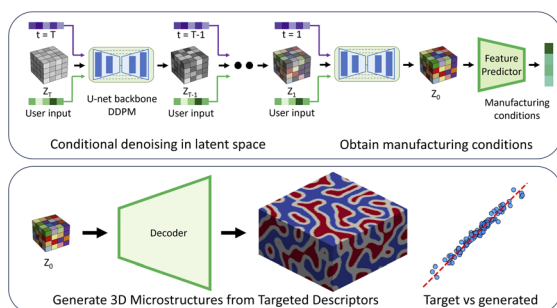
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The 2D-drone swarm, a safe open-source sample transfer system for fully automated laboratories

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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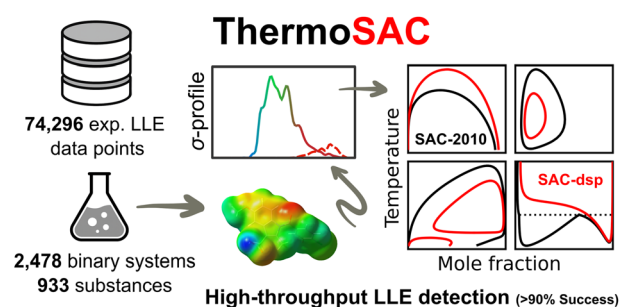
3D multiphase heterogeneous microstructure generation using conditional latent diffusion models

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



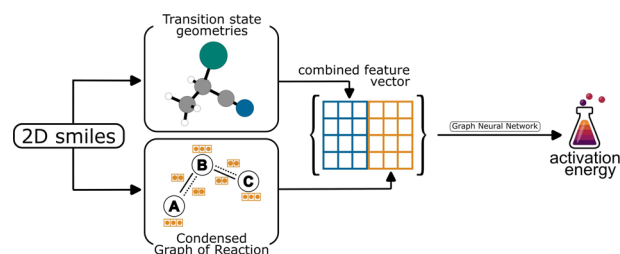
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High-throughput application and evaluation of the COSMO-SAC model for predictions of liquid–liquid equilibria

Ivan Antolović, Simon Stephan and Jadran Vrabc*^{*}

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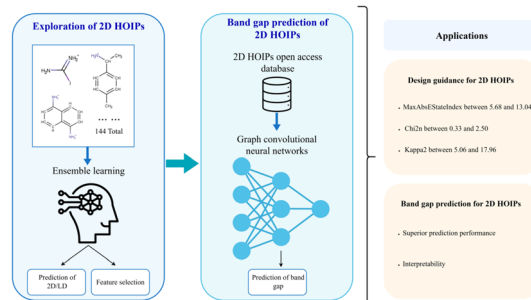
Graph-based prediction of reaction barrier heights with on-the-fly prediction of transition states

Johannes Karwounopoulos, Jasper De Landsheere, Leonard Galustian, Tobias Jechtl and Esther Heid*^{*}

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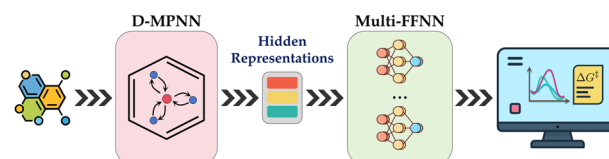
Design guidance and band gap prediction of two-dimensional hybrid organic–inorganic perovskites by ensemble learning and graph convolutional neural networks

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

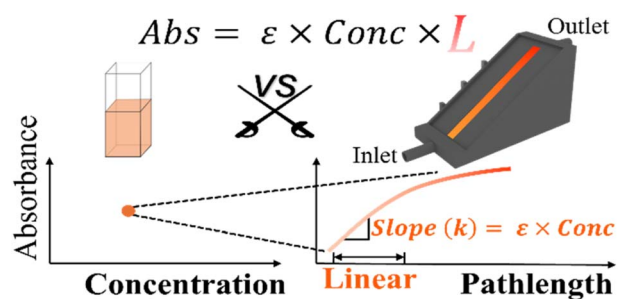


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Harnessing surrogate models for data-efficient predictive chemistry: descriptors vs. learned hidden representations

Guanming Chen and Thijs Stuyver*^{*}

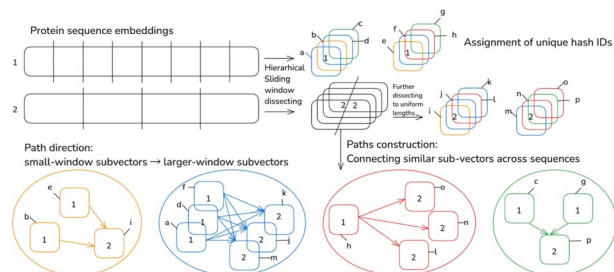
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Variable pathlength cell for internal data validation in computer vision

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

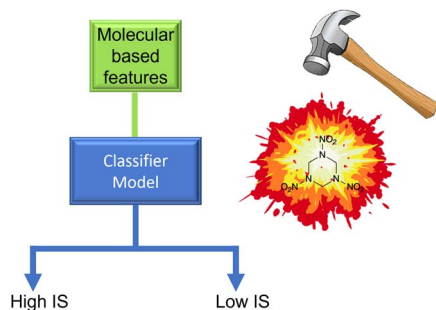
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MAAPE: a tool for modular evolution analysis of protein embeddings

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

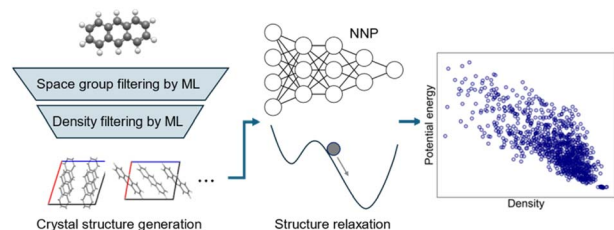
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Understanding impact sensitivity of energetic molecules by supervised machine learning

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

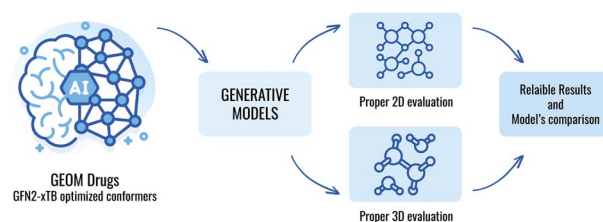
Takuya Taniguchi* and Ryo Fukasawa



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

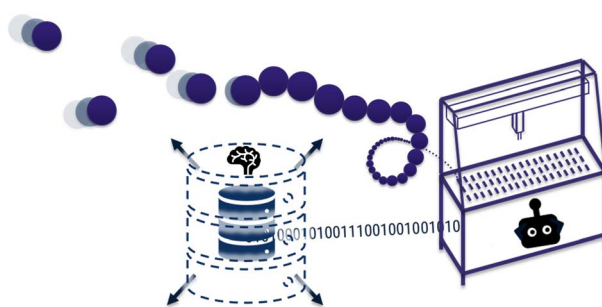
Filipp Nikitin, Ian Dunn, David Ryan Koes and Olexandr Isayev*



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

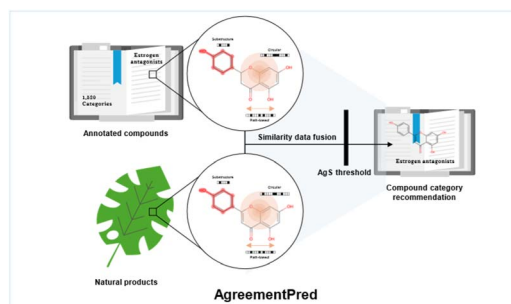
Michael Ringleb, Yannik Köster, Stefan Zechel and Ulrich S. Schubert*



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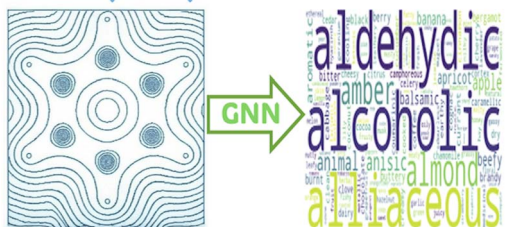
Optimal message passing for molecular prediction is simple, attentive and spatial

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



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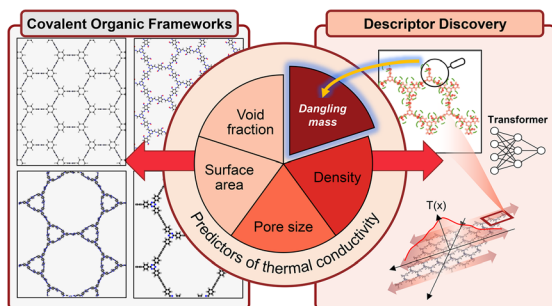
DenseSense: Machine learning based perception of scent



Dense Sense: a novel approach utilizing electron density augmented machine learning paradigm to understand the complex odour landscape

Pinaki Saha,* Mrityunjay Sharma, Sarabeshwar Balaji, Aryan Amit Barsainyan, Ritesh Kumar,* Volker Steuber and Michael Schmuker

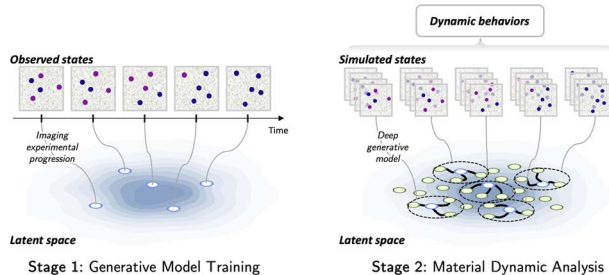
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Deep learning reveals key predictors of thermal conductivity in covalent organic frameworks

Prakash Thakolkaran, Yiwen Zheng, Yaqi Guo, Aniruddh Vashisth* and Siddhant Kumar*

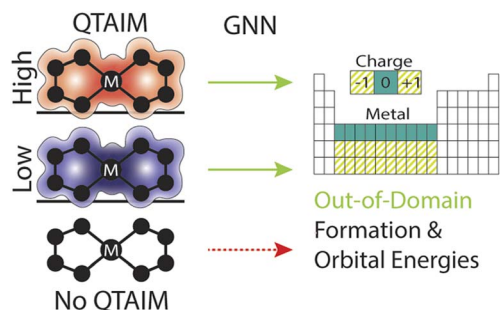
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Material dynamics analysis with deep generative model

Duc-Anh Dao, Minh-Quyet Ha, Tien-Sinh Vu, Shuntaro Takazawa, Nozomu Ishiguro, Yukio Takahashi, Suzuki Masato, Takashi Kakubo, Naoya Amino, Hirotsuke Matsui, Mizuki Tada and Hieu-Chi Dam*

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Multi-level QTAIM-enriched graph neural networks for resolving properties of transition metal complexes

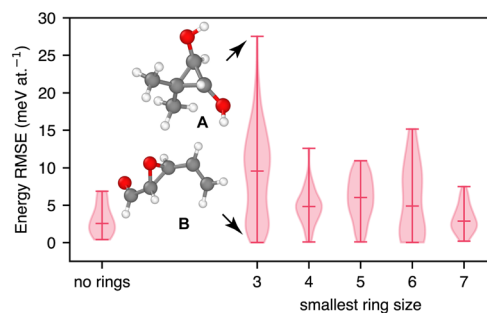
Winston Gee, Abigail Doyle, Santiago Vargas* and Anastassia N. Alexandrova*



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

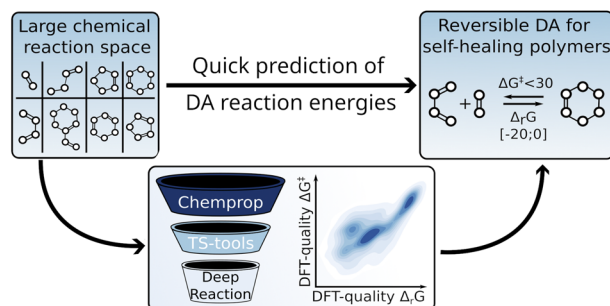
Chiheb Ben Mahmoud,* Zakariya El-Machachi, Krystian A. Gierczak, John L. A. Gardner and Volker L. Deringer



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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*



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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*

