

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 DDIAI 4(1) 1–290 (2025)



Cover
See Arash Khajeh *et al.*, pp. 11–20. Image reproduced by permission of the Toyota Research Institute from *Digital Discovery*, 2025, 4, 11.



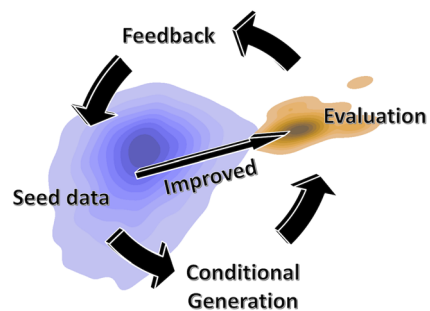
Inside cover
See Masahiko Taniguchi and Jonathan S. Lindsey, pp. 21–34. Image reproduced by permission of Masahiko Taniguchi from *Digital Discovery*, 2025, 4, 21.

PAPERS

11

A materials discovery framework based on conditional generative models applied to the design of polymer electrolytes

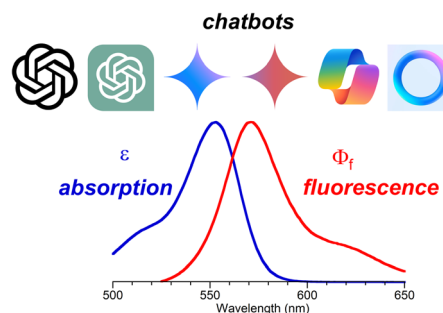
Arash Khajeh,* Xiangyun Lei, Weike Ye, Zhenze Yang, Linda Hung, Daniel Schweigert and Ha-Kyung Kwon



21

Acquisition of absorption and fluorescence spectral data using chatbots

Masahiko Taniguchi* and Jonathan S. Lindsey



**GOLD
OPEN
ACCESS**

EES Batteries

**Exceptional research on
batteries and energy storage**

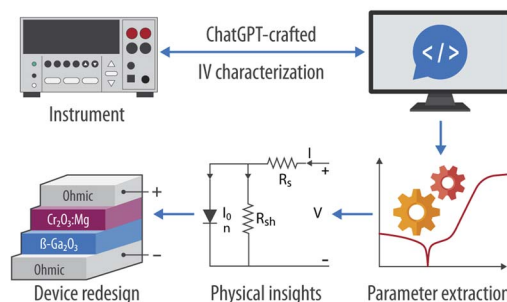
Part of the EES family

**Join
in** | Publish with us
rsc.li/EESBatteries

35

From text to test: AI-generated control software for materials science instruments

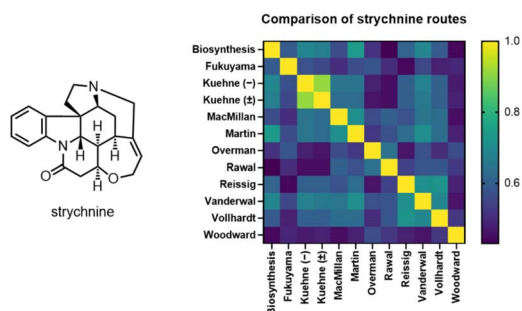
Davi Fébba, Kingsley Egbo, William A. Callahan and Andriy Zakutayev



46

A simple similarity metric for comparing synthetic routes

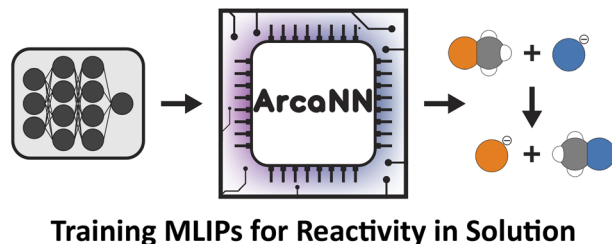
Samuel Genheden* and Jason D. Shields*



54

ArcaNN: automated enhanced sampling generation of training sets for chemically reactive machine learning interatomic potentials

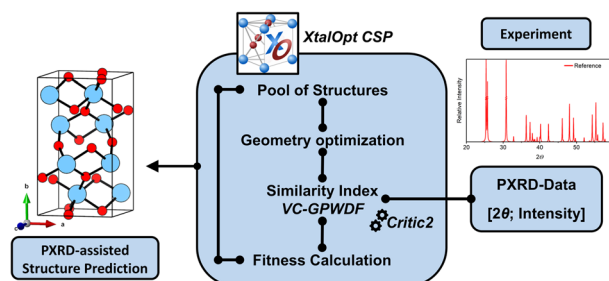
Rolf David,* Miguel de la Puente, Axel Gomez, Olaia Anton, Guillaume Stirnemann* and Damien Laage*



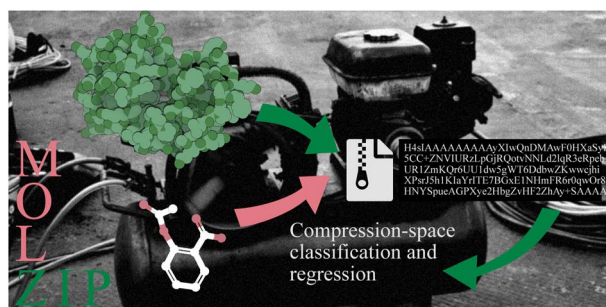
73

Powder X-ray diffraction assisted evolutionary algorithm for crystal structure prediction

Stefano Racioppi, Alberto Otero-de-la-Roza, Samad Hajinazar and Eva Zurek*



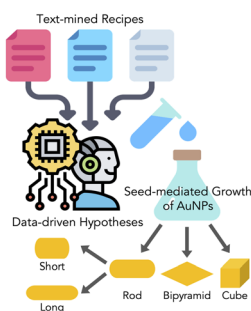
84



Learning on compressed molecular representations

Jan Weinreich and Daniel Probst*

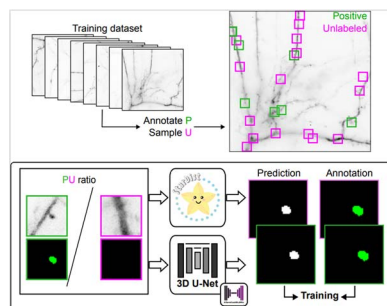
93



Data-driven analysis of text-mined seed-mediated syntheses of gold nanoparticles

Sanghoon Lee, Kevin Cruse, Samuel P. Gleason, A. Paul Alivisatos, Gerbrand Ceder and Anubhav Jain*

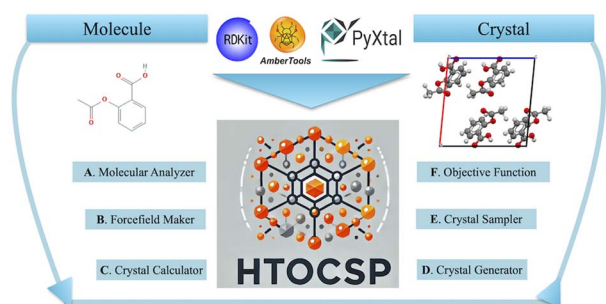
105



Quantitative analysis of miniature synaptic calcium transients using positive unlabeled deep learning

Frédéric Beaupré, Anthony Bilodeau, Theresa Wiesner, Gabriel Leclerc, Mado Lemieux, Gabriel Nadeau, Katrine Castonguay, Bolin Fan, Simon Labrecque, Renée Hložek, Paul De Koninck, Christian Gagné and Flavie Lavoie-Cardinal*

120



Automated high-throughput organic crystal structure prediction via population-based sampling

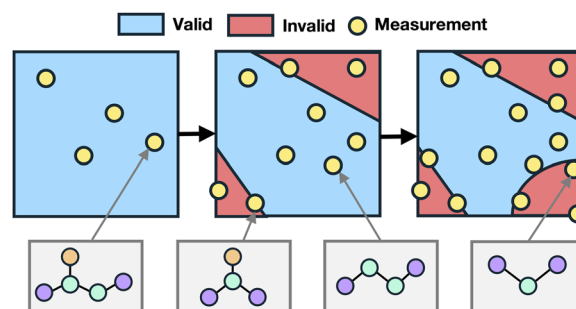
Qiang Zhu* and Shinnosuke Hattori*



135

Data efficiency of classification strategies for chemical and materials design

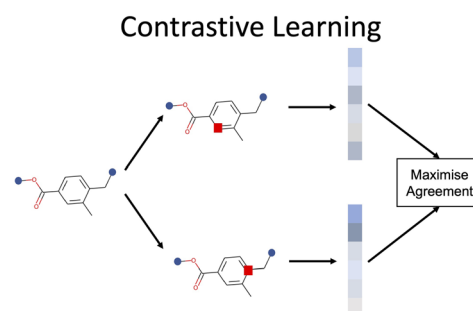
Quinn M. Gallagher and Michael A. Webb*



149

PolyCL: contrastive learning for polymer representation learning *via* explicit and implicit augmentations

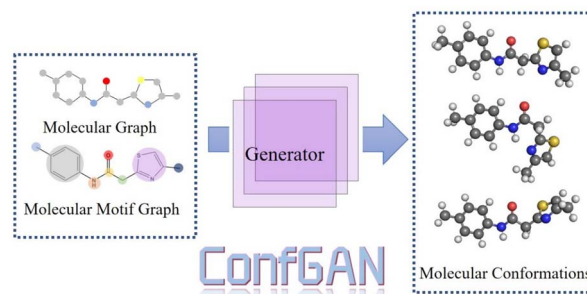
Jiajun Zhou, Yijie Yang, Austin M. Mroz and Kim E. Jelfs*



161

Generation of molecular conformations using generative adversarial networks

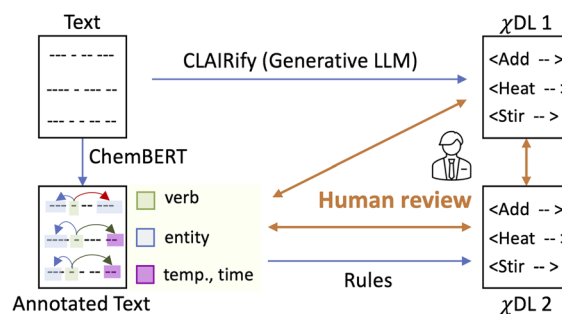
Congsheng Xu, Xiaomei Deng, Yi Lu and Peiyuan Yu*



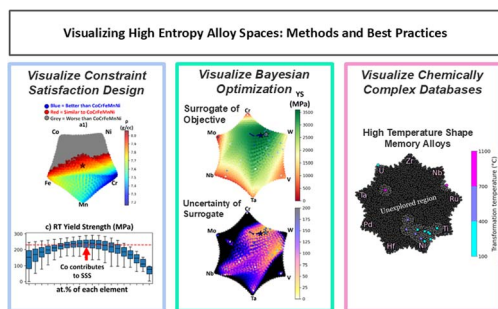
172

A framework for reviewing the results of automated conversion of structured organic synthesis procedures from the literature

Kojiro Machi,* Seiji Akiyama, Yuuya Nagata and Masaharu Yoshioka*



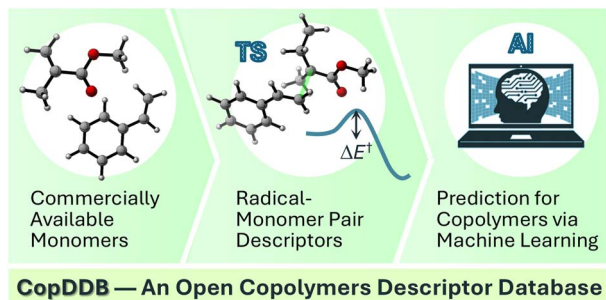
181



Visualizing high entropy alloy spaces: methods and best practices

Brent Vela, Trevor Hastings,* Marshall Allen and Raymundo Arróyave

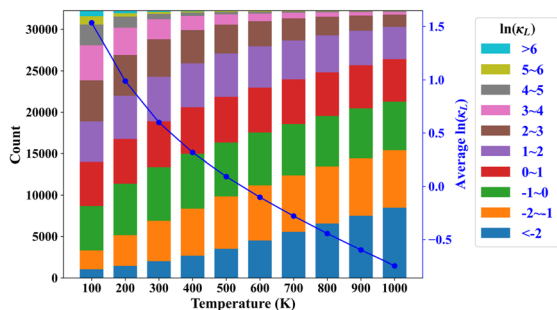
195



CopDDB: a descriptor database for copolymers and its applications to machine learning

Takayoshi Yoshimura, Hiromoto Kato, Shunto Oikawa, Taichi Inagaki, Shigehito Asano, Tetsunori Sugawara, Tomoyuki Miyao, Takamitsu Matsubara, Hiroharu Ajiro, Mikiya Fujii, Yu-ya Ohnishi and Miho Hatanaka*

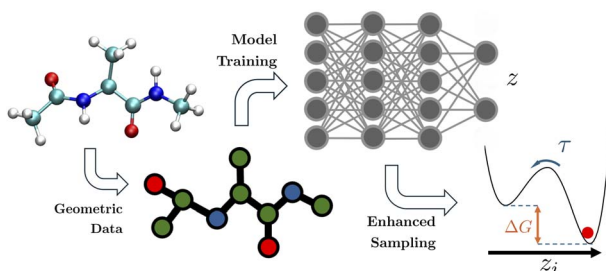
204



Machine learning for accelerated prediction of lattice thermal conductivity at arbitrary temperature

Zihe Li, Mengke Li, Yufeng Luo, Haibin Cao, Huijun Liu* and Ying Fang*

211



A graph neural network-state predictive information bottleneck (GNN-SPIB) approach for learning molecular thermodynamics and kinetics

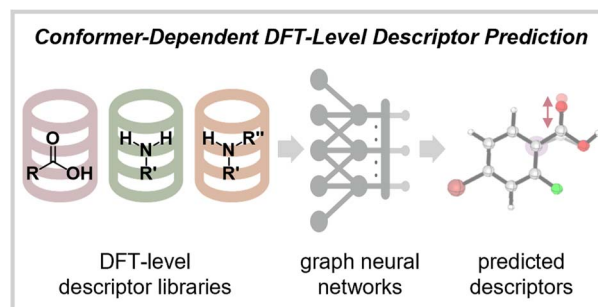
Ziyue Zou, Dedi Wang and Pratyush Tiwary*



222

Rapid prediction of conformationally-dependent DFT-level descriptors using graph neural networks for carboxylic acids and alkyl amines

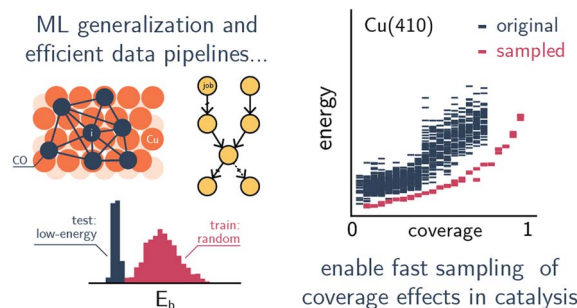
Brittany C. Haas, Melissa A. Hardy, Shree Sowndarya S. V., Keir Adams, Connor W. Coley,* Robert S. Paton* and Matthew S. Sigman*



234

Comprehensive sampling of coverage effects in catalysis by leveraging generalization in neural network models

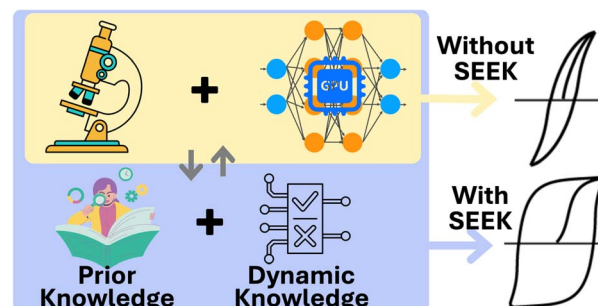
Daniel Schwalbe-Koda,* Nitish Govindarajan* and Joel B. Varley



252

Scientific exploration with expert knowledge (SEEK) in autonomous scanning probe microscopy with active learning

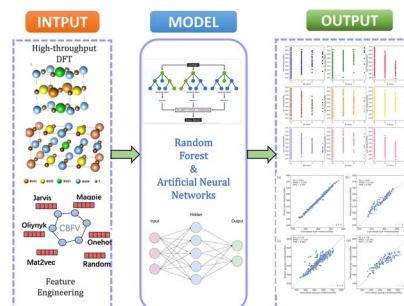
Utkarsh Pratiush, Hiroshi Funakubo, Rama Vasudevan, Sergei V. Kalinin* and Yongtao Liu*

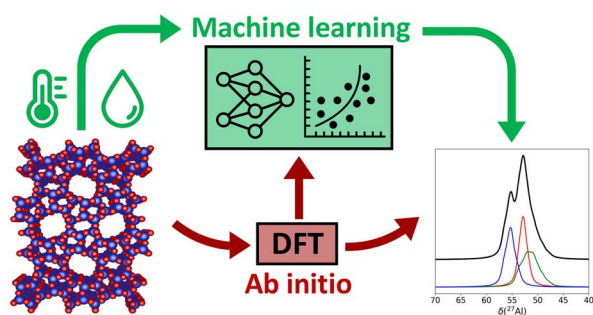


264

Predicting mechanical properties of non-equimolar high-entropy carbides using machine learning

Xi Zhao,* Shu-guang Cheng, Sen Yu, Jiming Zheng, Rui-Zhi Zhang and Meng Guo





^{27}Al NMR chemical shifts in zeolite MFI via machine learning acceleration of structure sampling and shift prediction

Daniel Willimetz,^{*} Andreas Erlebach, Christopher J. Heard and Lukáš Grajciar^{*}

