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

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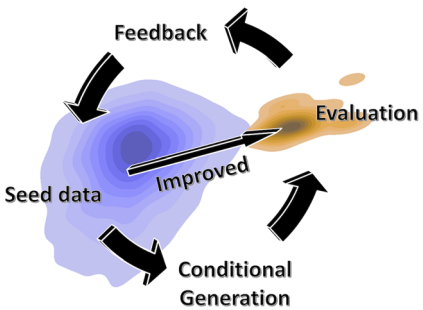
A materials discovery framework based on conditional generative models applied to the design of polymer electrolytes

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



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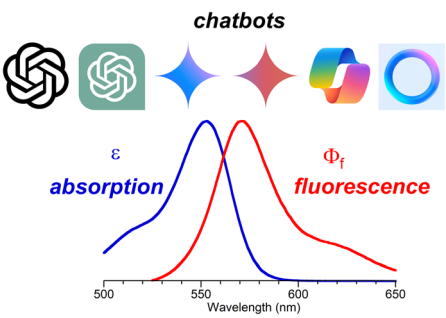
Acquisition of absorption and fluorescence spectral data using chatbots

Masahiko Taniguchi* and Jonathan S. Lindsey



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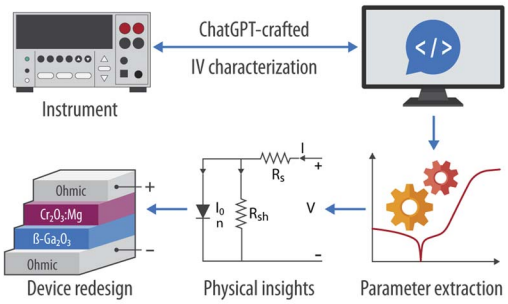
From text to test: AI-generated control software for materials science instruments

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



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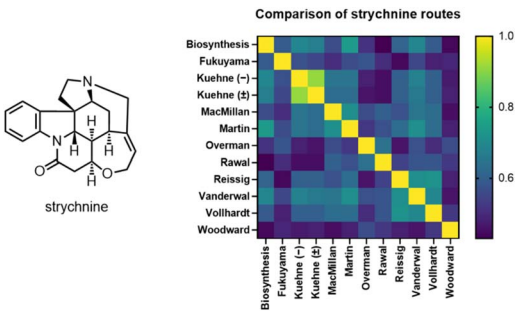
A simple similarity metric for comparing synthetic routes

Samuel Genheden* and Jason D. Shields*



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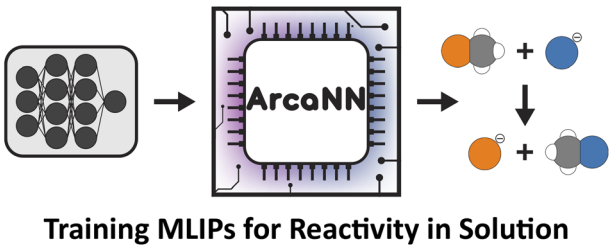
ArcaNN: automated enhanced sampling generation of training sets for chemically reactive machine learning interatomic potentials

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



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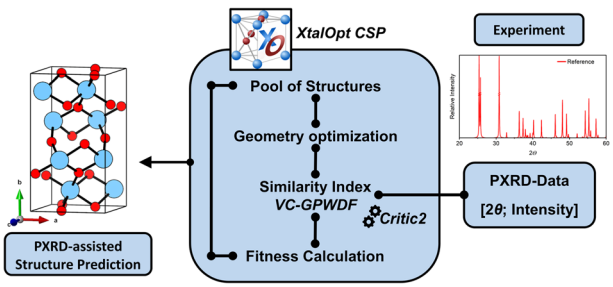
Powder X-ray diffraction assisted evolutionary algorithm for crystal structure prediction

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



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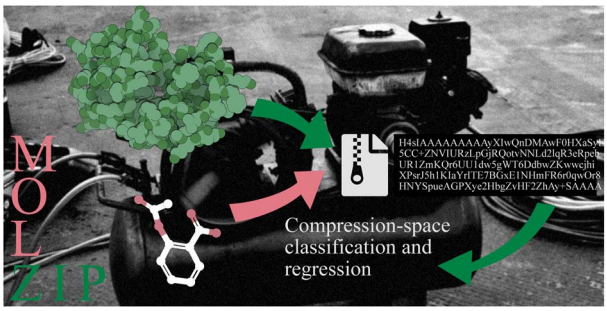

Learning on compressed molecular representations

Jan Weinreich and Daniel Probst*

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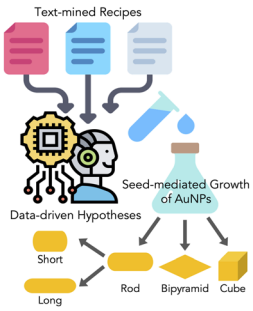

Data-driven analysis of text-mined seed-mediated syntheses of gold nanoparticles

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

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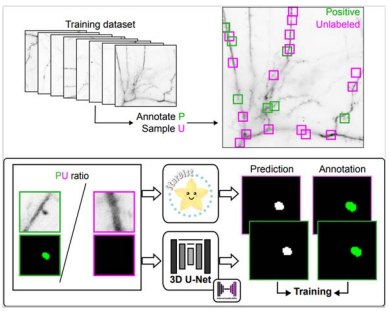

Quantitative analysis of miniature synaptic calcium transients using positive unlabeled deep learning

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*

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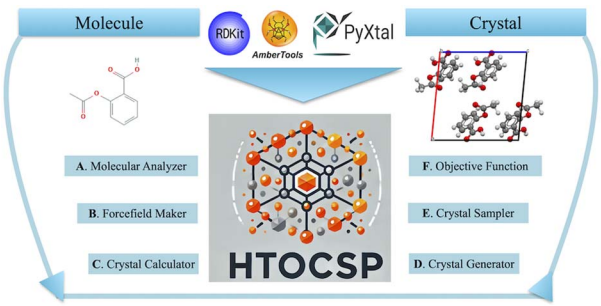

Automated high-throughput organic crystal structure prediction *via* population-based sampling

Qiang Zhu* and Shinnosuke Hattori*

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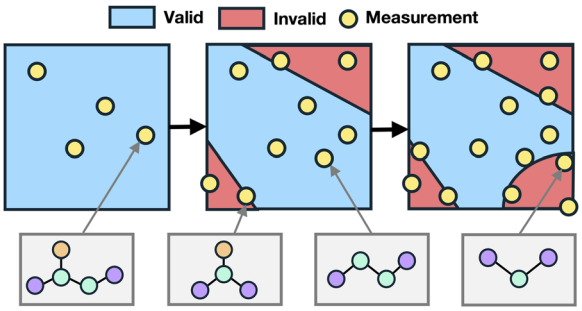
Data efficiency of classification strategies for chemical and materials design

Quinn M. Gallagher and Michael A. Webb*



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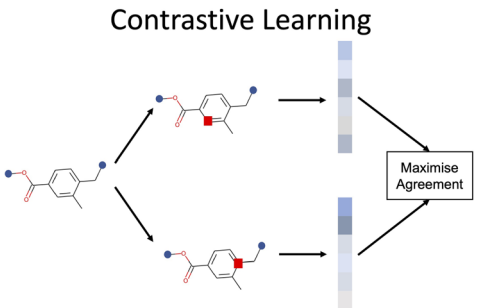
PolyCL: contrastive learning for polymer representation learning *via* explicit and implicit augmentations

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



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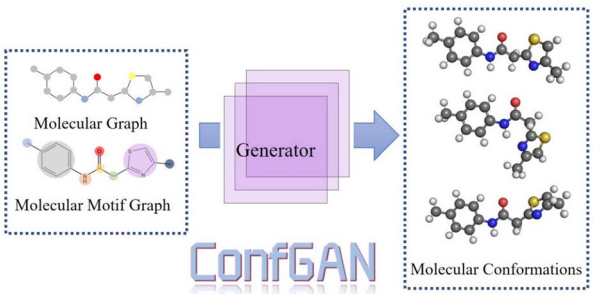
Generation of molecular conformations using generative adversarial neural networks

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



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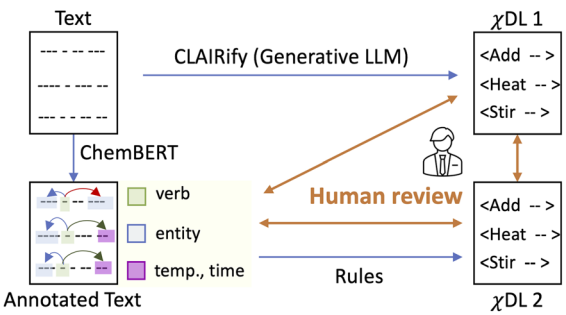
A framework for reviewing the results of automated conversion of structured organic synthesis procedures from the literature

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



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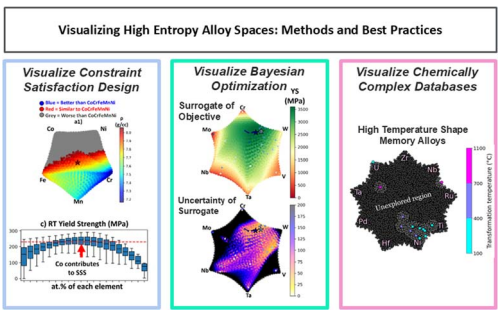

Visualizing high entropy alloy spaces: methods and best practices

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

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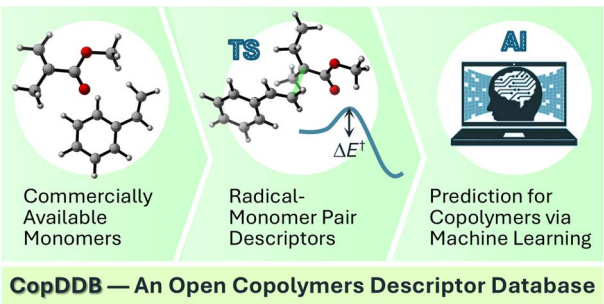

CopDDB: a descriptor database for copolymers and its applications to machine learning

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*

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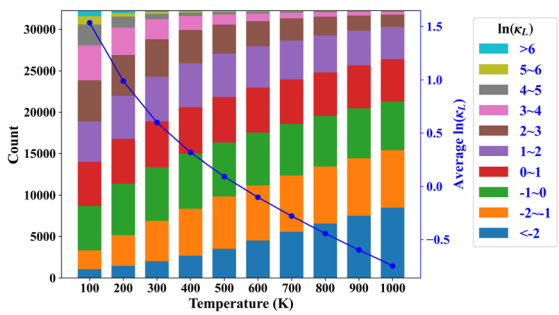

Machine learning for accelerated prediction of lattice thermal conductivity at arbitrary temperature

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

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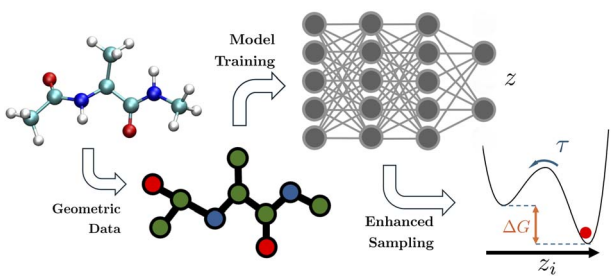

A graph neural network-state predictive information bottleneck (GNN-SPIB) approach for learning molecular thermodynamics and kinetics

Ziyue Zou, Dedi Wang and Pratyush Tiwary*

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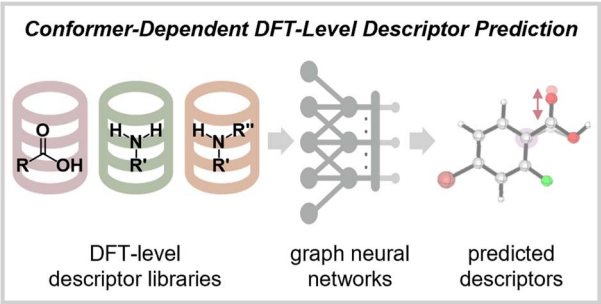
Rapid prediction of conformationally-dependent DFT-level descriptors using graph neural networks for carboxylic acids and alkyl amines

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



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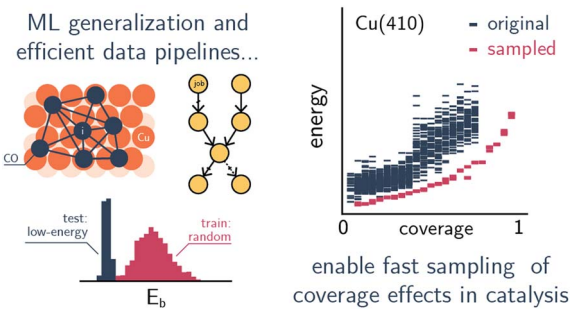
Comprehensive sampling of coverage effects in catalysis by leveraging generalization in neural network models

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



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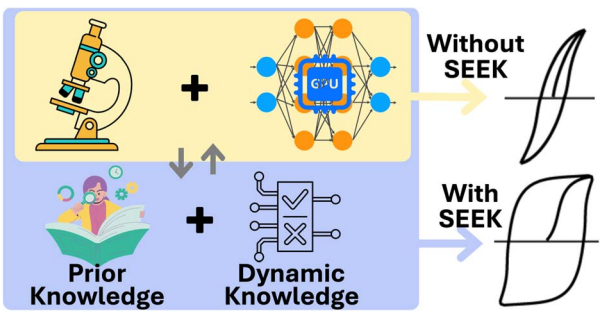
Scientific exploration with expert knowledge (SEEK) in autonomous scanning probe microscopy with active learning

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



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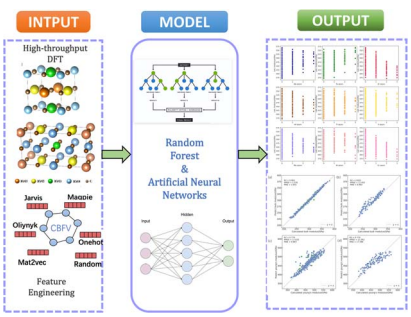
Predicting mechanical properties of non-equimolar high-entropy carbides using machine learning

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



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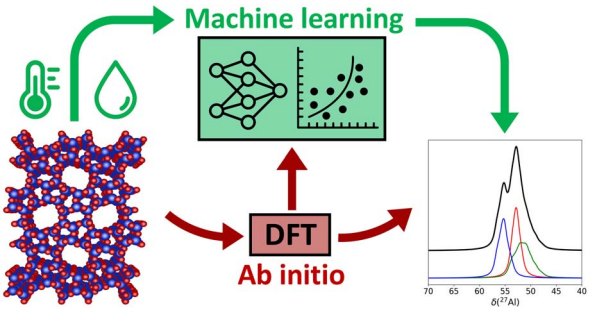

^{27}Al NMR chemical shifts in zeolite MFI *via* machine learning acceleration of structure sampling and shift prediction

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

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