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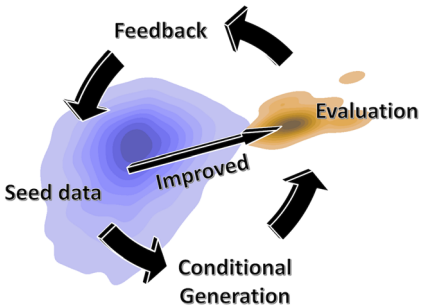

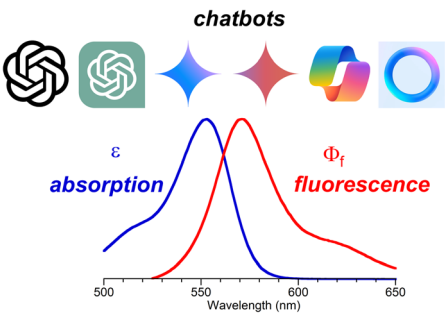

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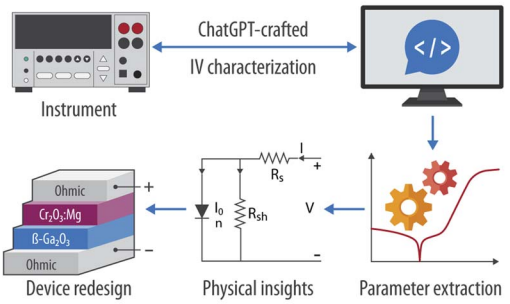
From text to test: AI-generated control software for materials science instruments

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



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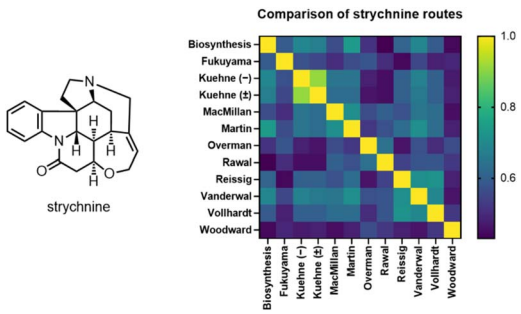
A simple similarity metric for comparing synthetic routes

Samuel Genheden* and Jason D. Shields*



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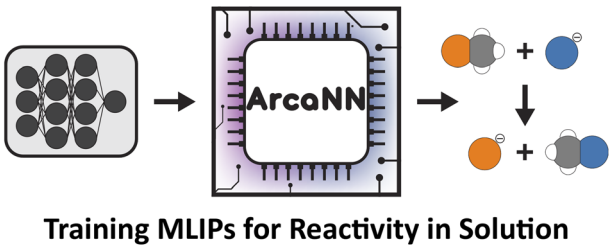
ArcaNN: automated enhanced sampling generation of training sets for chemically reactive machine learning interatomic potentials

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



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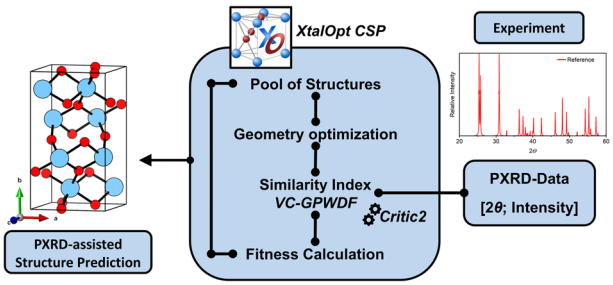
Powder X-ray diffraction assisted evolutionary algorithm for crystal structure prediction

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



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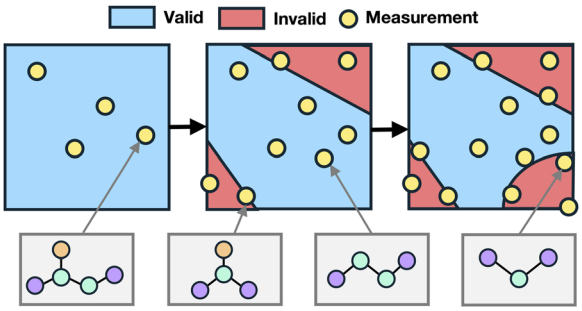

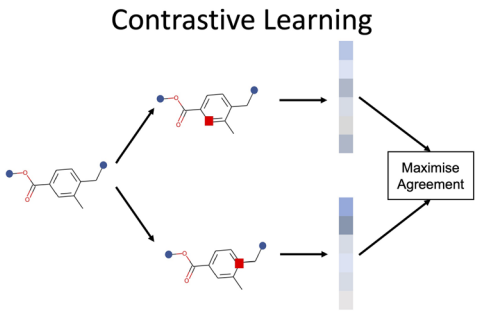

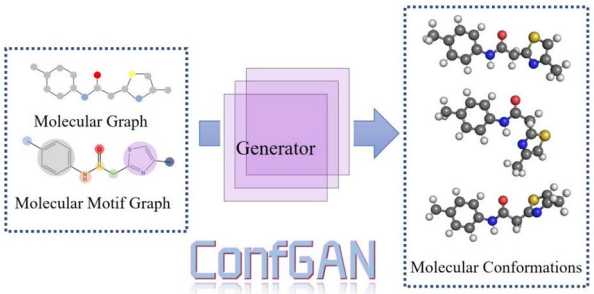

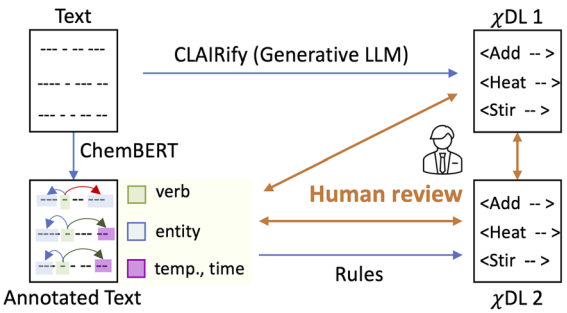

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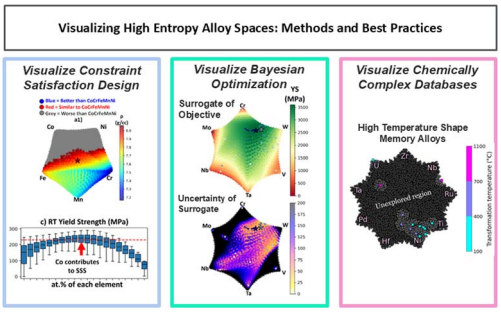

Visualizing high entropy alloy spaces: methods and best practices

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

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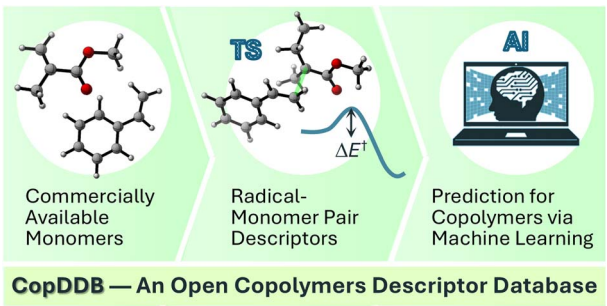

CopDDB: a descriptor database for copolymers and its applications to machine learning

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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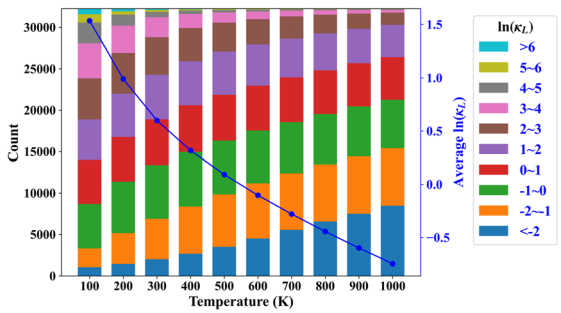

Machine learning for accelerated prediction of lattice thermal conductivity at arbitrary temperature

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

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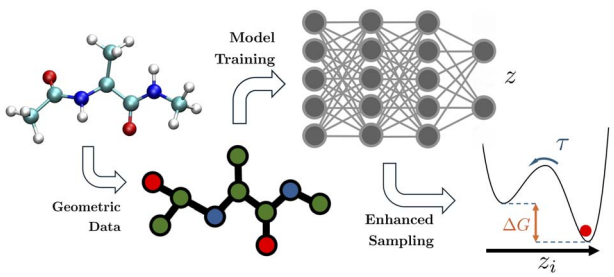

A graph neural network-state predictive information bottleneck (GNN-SPIB) approach for learning molecular thermodynamics and kinetics

Ziyue Zou, Dedi Wang and Pratyush Tiwary*

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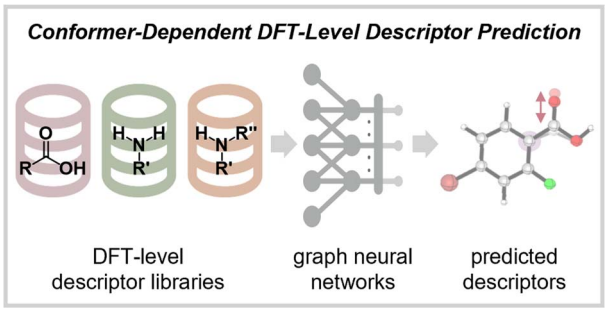
Rapid prediction of conformationally-dependent DFT-level descriptors using graph neural networks for carboxylic acids and alkyl amines

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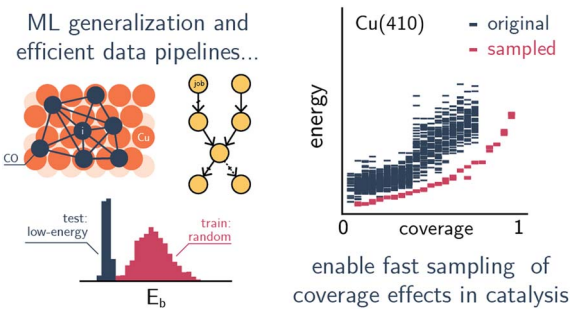
Comprehensive sampling of coverage effects in catalysis by leveraging generalization in neural network models

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



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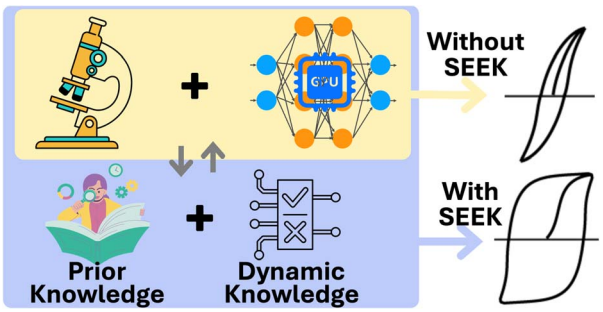
Scientific exploration with expert knowledge (SEEK) in autonomous scanning probe microscopy with active learning

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



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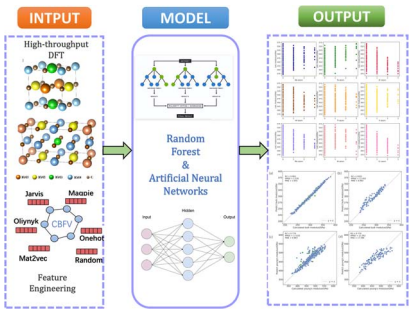
Predicting mechanical properties of non-equimolar high-entropy carbides using machine learning

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



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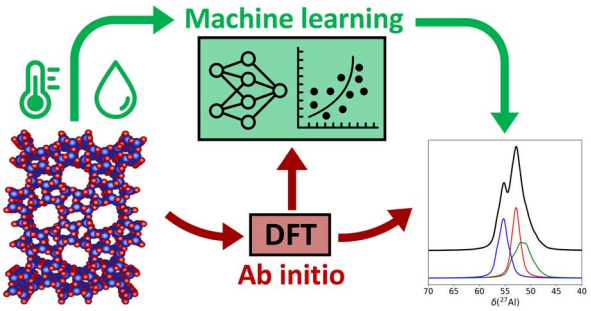

^{27}Al NMR chemical shifts in zeolite MFI *via* machine learning acceleration of structure sampling and shift prediction

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

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