

## IN THIS ISSUE

ISSN 2635-098X CODEN DDIAI 3(11) 2149–2386 (2024)



### Cover

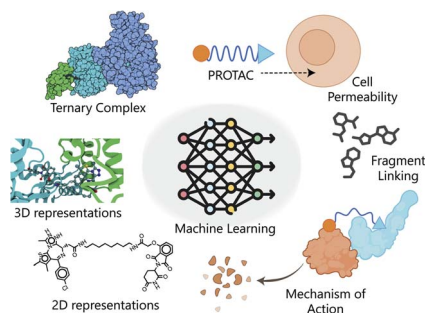
See Chen Ling *et al.*, pp. 2183–2191. Image reproduced by permission of Chen Ling from *Digital Discovery*, 2024, **3**, 2183.

## REVIEW

2158

### A comprehensive review of emerging approaches in machine learning for *de novo* PROTAC design

Yossra Gharbi and Rocío Mercado\*

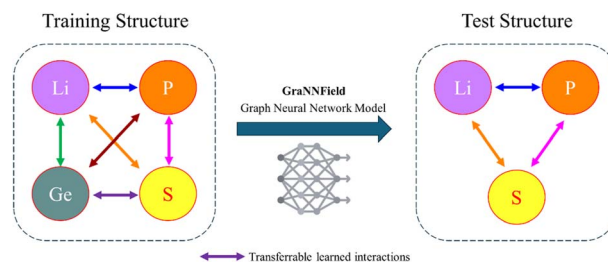


## COMMUNICATION

2177

### Stability and transferability of machine learning force fields for molecular dynamics applications

Salatan Duangdangchote, Dwight S. Seferos and Oleksandr Voznyy\*



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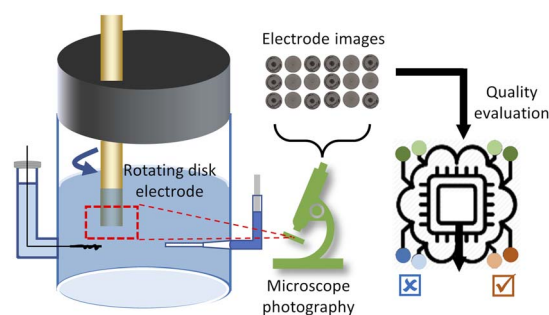
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## Computer vision enabled high-quality electrochemical experimentation

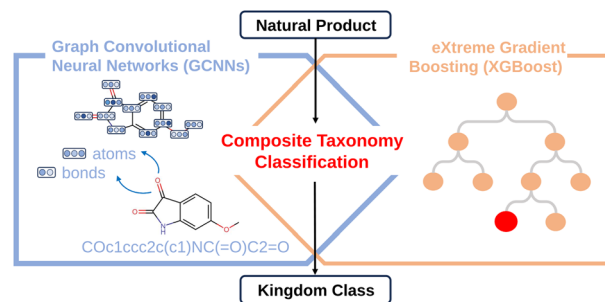
Keiichi Okubo, Jaydeep Thik, Tomoya Yamaguchi and Chen Ling\*



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## Composite machine learning strategy for natural products taxonomical classification and structural insights

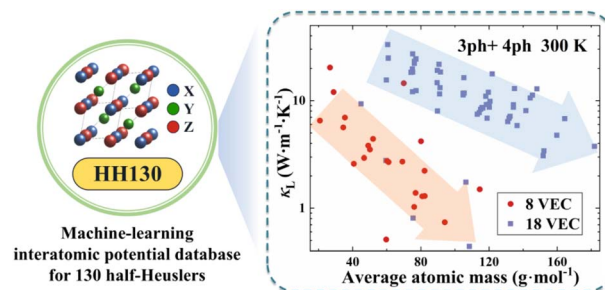
Qisong Xu, Alan K. X. Tan, Liangfeng Guo, Yee Hwee Lim, Dillon W. P. Tay\* and Shi Jun Ang\*



2201

## HH130: a standardized database of machine learning interatomic potentials, datasets, and its applications in the thermal transport of half-Heusler thermoelectrics

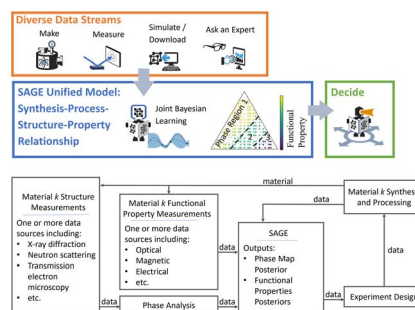
Yuyan Yang, Yifei Lin, Shengnan Dai,\* Yifan Zhu, Jinyang Xi, Lili Xi, Xiaokun Gu, David J. Singh, Wenqing Zhang and Jiong Yang\*



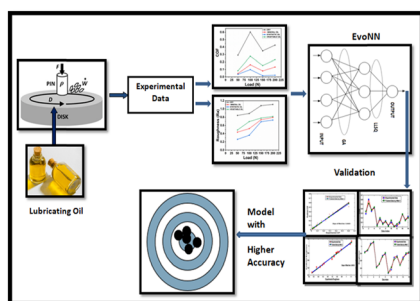
2211

## Learning material synthesis–process–structure–property relationship by data fusion: Bayesian co-regionalization N-dimensional piecewise function learning

A. Gilad Kusne,\* Austin McDannald and Brian DeCost



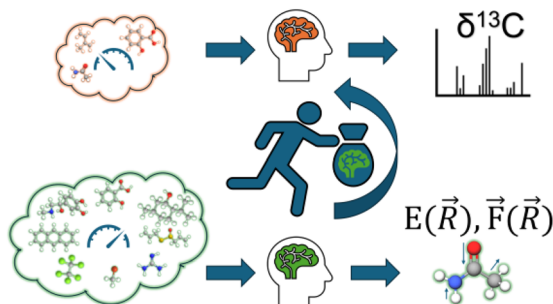
2226



### Machine learning-assisted analysis of dry and lubricated tribological properties of Al–Co–Cr–Fe–Ni high entropy alloy

Saurabh Vashistha, Bashista Kumar Mahanta, Vivek Kumar Singh, Neha Sharma, Anjan Ray, Saurabh Dixit and Shailesh Kumar Singh\*

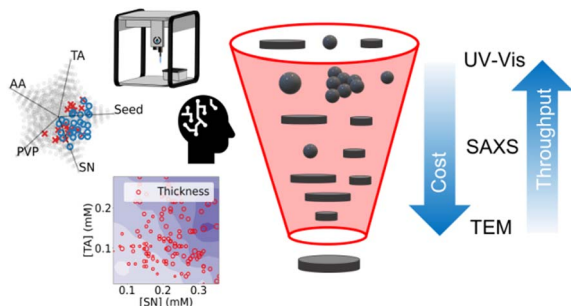
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### Transfer learning based on atomic feature extraction for the prediction of experimental $^{13}\text{C}$ chemical shifts

Žarko Ivković, Jesús Jover and Jeremy Harvey

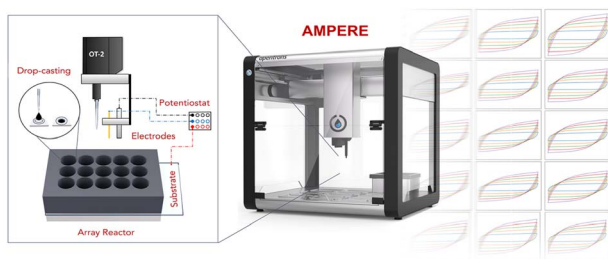
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### Data-driven exploration of silver nanoplate formation in multidimensional chemical design spaces

Huat Thart Chiang,\* Kiran Vaddi and Lilo Pozzo\*

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### AMPERE: automated modular platform for expedited and reproducible electrochemical testing

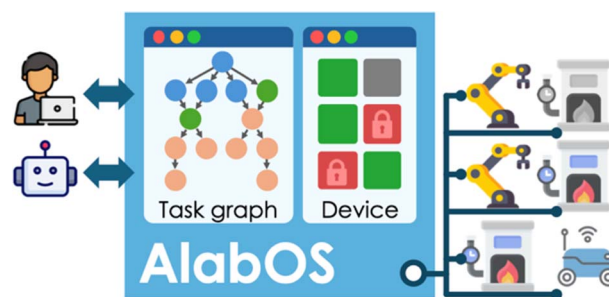
Jehad Abed, Yang Bai, Daniel Persaud, Jiheon Kim, Julia Witt, Jason Hattrick-Simpers\* and Edward H. Sargent\*



2275

### AlabOS: a Python-based reconfigurable workflow management framework for autonomous laboratories

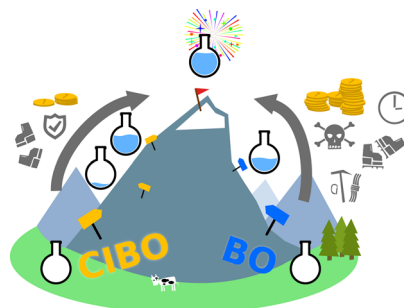
Yuxing Fei, Bernardus Rendy, Rishi Kumar, Olympia Dartsis, Hrushikesh P. Sahasrabudde, Matthew J. McDermott, Zheren Wang, Nathan J. Szymanski, Lauren N. Walters, David Milsted, Yan Zeng,\* Anubhav Jain\* and Gerbrand Ceder\*



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### Cost-informed Bayesian reaction optimization

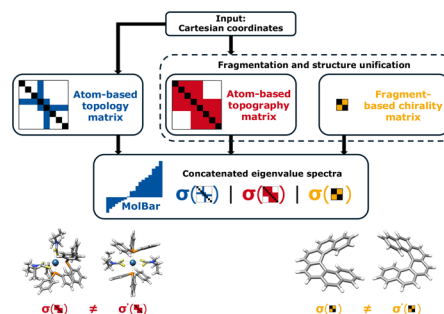
Alexandre A. Schoepfer, Jan Weinreich, Ruben Laplaza, Jerome Waser\* and Clemence Corminboeuf\*



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### MolBar: a molecular identifier for inorganic and organic molecules with full support of stereoisomerism

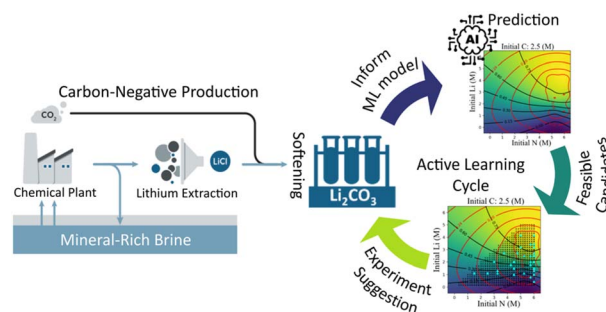
Nils van Staalduijn and Christoph Bannwarth\*



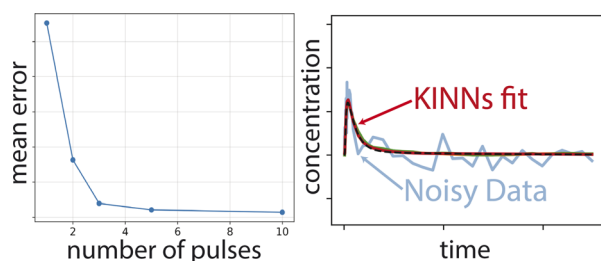
2320

### Artificial intelligence-enabled optimization of battery-grade lithium carbonate production

S. Shayan Mousavi Masouleh, Corey A. Sanz, Ryan P. Jansonius, Samuel Shi, Maria J. Gendron Romero, Jason E. Hein and Jason Hatrick-Simpers\*



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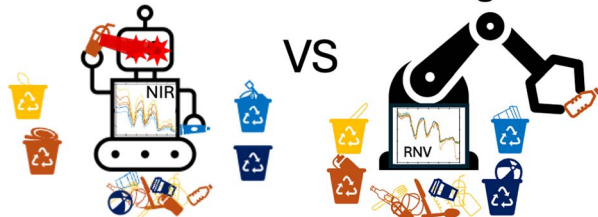


### Micro-kinetic modeling of temporal analysis of products data using kinetics-informed neural networks

Dingqi Nai, Gabriel S. Gusmão, Zachary A. Kilwein, Fani Boukouvala and Andrew J. Medford\*

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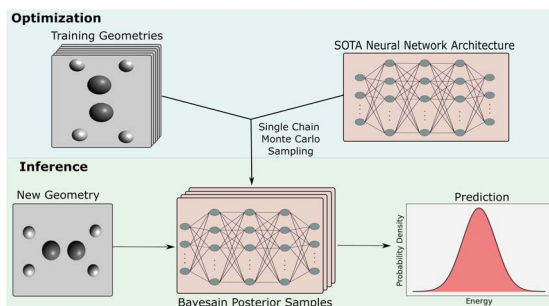
### Optimized Sorting of Polyolefins with Machine Learning



### Sorting polyolefins with near-infrared spectroscopy: identification of optimal data analysis pipelines and machine learning classifiers

Bradley P. Sutliff, Peter A. Beaucage, Debra J. Audus, Sara V. Orski and Tyler B. Martin\*

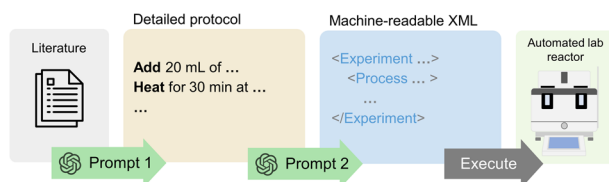
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### High accuracy uncertainty-aware interatomic force modeling with equivariant Bayesian neural networks

Tim Rensmeyer,\* Ben Craig, Denis Kramer and Oliver Niggemann

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### Leveraging GPT-4 to transform chemistry from paper to practice

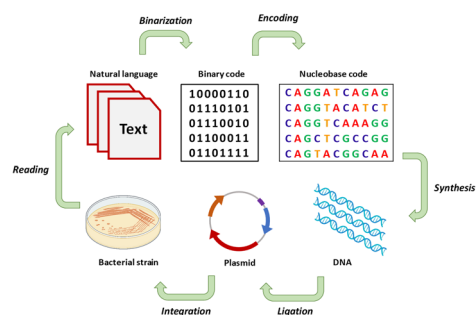
Wenyu Zhang, Mason A. Guy, Jerrica Yang, Lucy Hao, Junliang Liu, Joel M. Hawkins, Jason Mustakis, Sebastien Monfette\* and Jason E. Hein\*



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## Embedding DNA-based natural language in microbes for the benefit of future researchers

Heqian Zhang, Jiaquan Huang, Xiaoyu Wang, Zhizeng Gao, Song Meng, Hang Li, Shanshan Zhou, Shang Wang, Shan Wang, Xunyou Yan, Xinwei Yang, Xiaoluo Huang\* and Zhiwei Qin\*



## CORRECTION

2384

## Correction: A smile is all you need: predicting limiting activity coefficients from SMILES with natural language processing

Benedikt Winter, Clemens Winter, Johannes Schilling and André Bardow\*

