

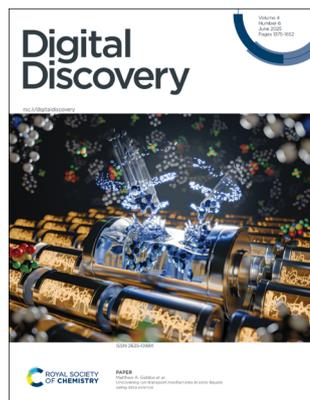
# Digital Discovery

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**Inside cover**  
See Philipp Benner *et al.*, pp. 1437–1448. Image reproduced by permission of Marie Maas from *Digital Discovery*, 2025, 4, 1437.

## PERSPECTIVE

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### Self-driving laboratories in Japan

Naruki Yoshikawa,\* Yuki Asano, Don N. Futaba, Kanako Harada, Taro Hitosugi, Genki N. Kanda, Shoichi Matsuda, Yuuya Nagata, Keisuke Nagato, Masanobu Naito, Tohru Natsume, Kazunori Nishio, Kanta Ono, Haruka Ozaki, Woosuck Shin, Junichiro Shiomi, Kunihiko Shizume, Koichi Takahashi, Seiji Takeda, Ichiro Takeuchi, Ryo Tamura, Koji Tsuda and Yoshitaka Ushiku

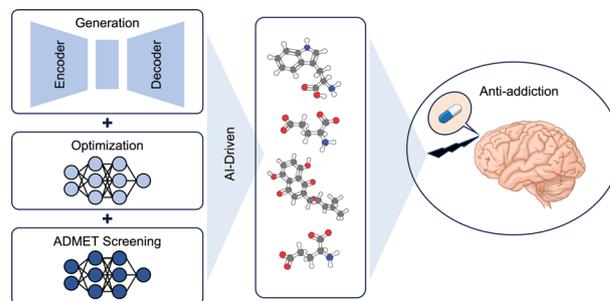


## REVIEW

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### Artificial intelligence approaches for anti-addiction drug discovery

Dong Chen, Jian Jiang, Nicole Hayes, Zhe Su and Guo-Wei Wei\*



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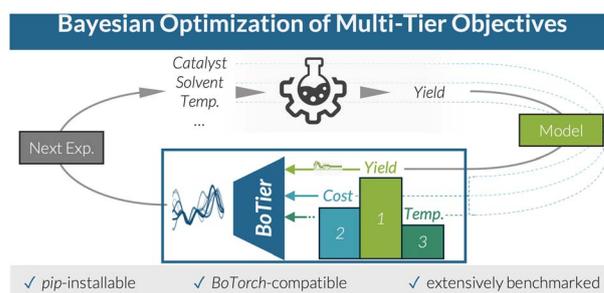
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### BoTier: multi-objective Bayesian optimization with tiered objective structures

Mohammad Haddadnia, Leonie Grashoff and Felix Strieth-Kalthoff\*

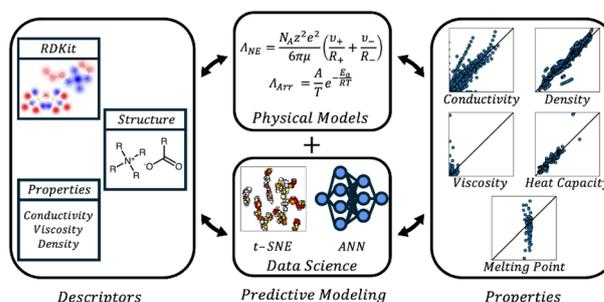


## PAPERS

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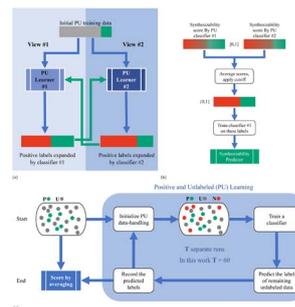
J. E. Umaña, Ryan K. Cashen, Victor M. Zavala and Matthew A. Gebbie\*



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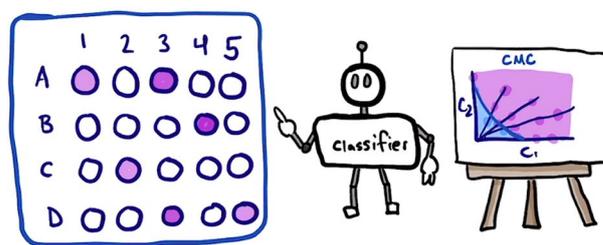
Sasan Amari Amir, Janine George and Philipp Benner\*



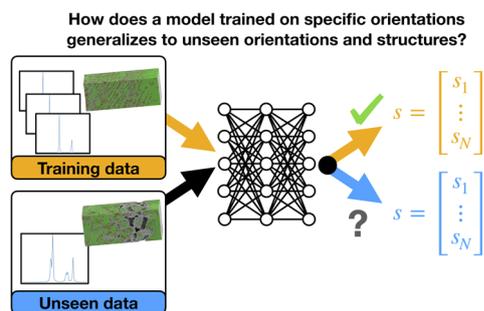
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### A classification-based methodology for the estimation of binary surfactant critical micelle concentrations

Chetan R. Chilkunda, John R. Kitchin and Robert D. Tilton\*



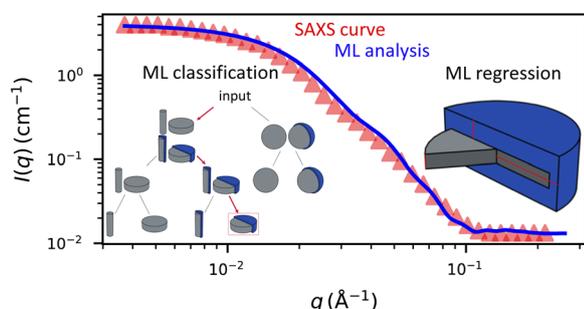
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### Exploring the transferability of machine-learning models for analyzing XRD data of shocked microstructures: from single crystal to polycrystals

Daniel Vizoso, Phillip Tsurkan, Ke Ma, Avinash M. Dongare and Rémi Dingreville\*

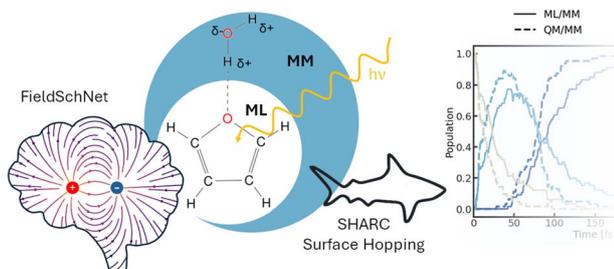
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### Automated structural analysis of small angle scattering data from common nanoparticles via machine learning

Graham Roberts, Mu-Ping Nieh, Anson W. K. Ma and Qian Yang\*

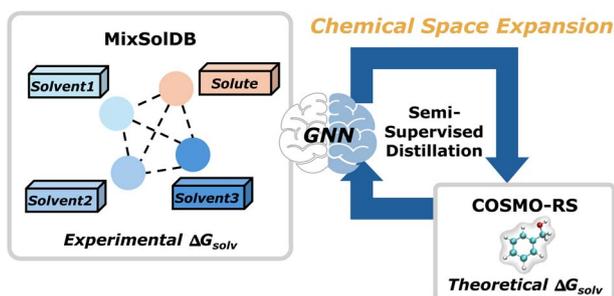
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### Excited-state nonadiabatic dynamics in explicit solvent using machine learned interatomic potentials

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### Enhancing predictive models for solubility in multicomponent solvent systems using semi-supervised graph neural networks

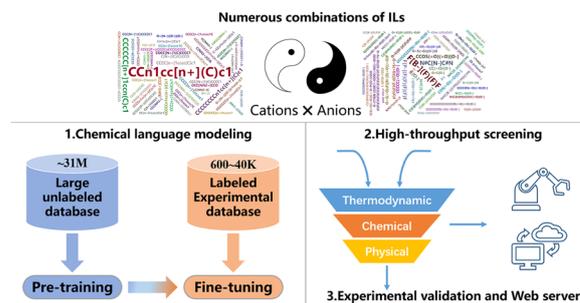
Hojin Jung, Christopher D. Stubbs, Sabari Kumar, Raúl Pérez-Soto, Su-min Song, Yeonjoon Kim\* and Seonah Kim\*



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## Large chemical language models for property prediction and high-throughput screening of ionic liquids

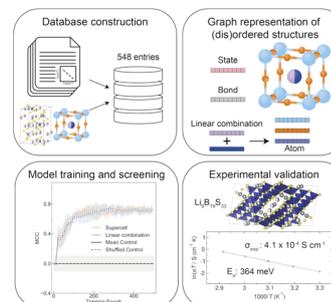
Yuxin Qiu, Zhen Song,<sup>\*</sup> Guzhong Chen, Wenyao Chen, Long Chen, Kake Zhu,<sup>\*</sup> Zhiwen Qi, Xuezhi Duan<sup>\*</sup> and De Chen



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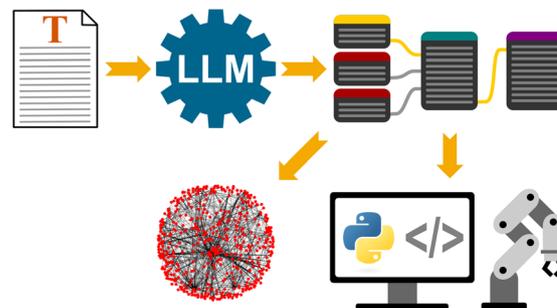
Daniel B. McHaffie, Zachery W. B. Iton, Jadon M. Bienz, Forrest A. L. Laskowski and Kimberly A. See<sup>\*</sup>



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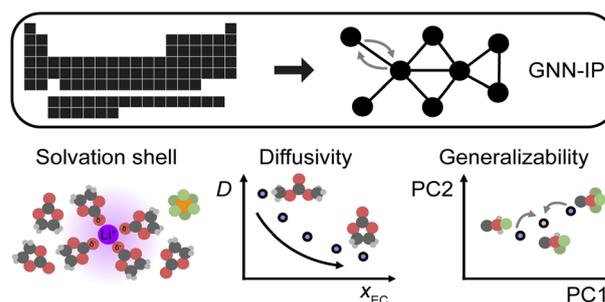
Bastian Ruehle<sup>\*</sup>



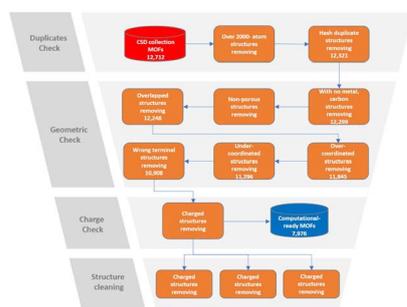
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## Application of pretrained universal machine-learning interatomic potential for physicochemical simulation of liquid electrolytes in Li-ion batteries

Suyeon Ju, Jinmu You, Gijin Kim, Yutack Park, Hyungmin An and Seungwu Han<sup>\*</sup>



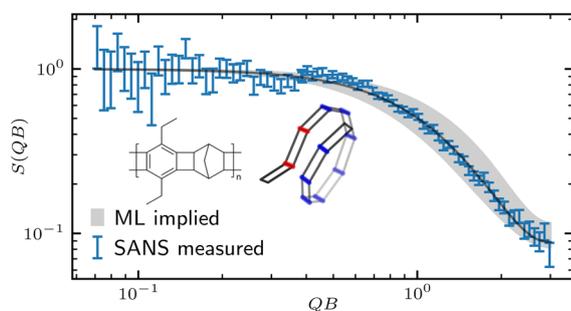
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Lijie Ding, Chi-Huan Tung, Zhiqiang Cao, Zekun Ye, Xiaodan Gu, Yan Xia, Wei-Ren Chen and Changwoo Do\*

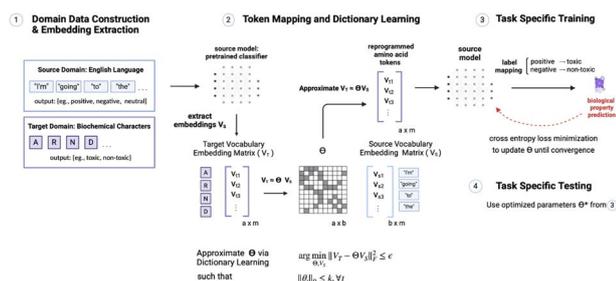
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Lei Zhang,\* Lars Banko, Wolfgang Schuhmann, Alfred Ludwig and Markus Stricker

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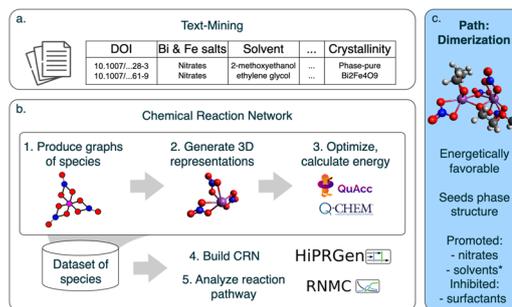
Ria Vinod, Pin-Yu Chen\* and Payel Das\*



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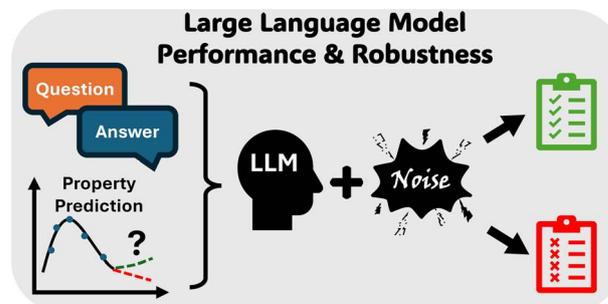
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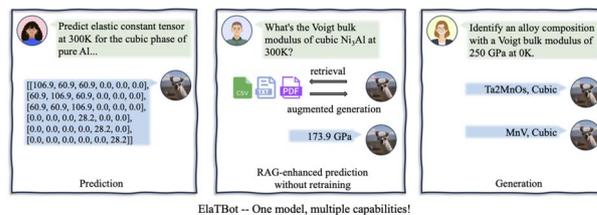
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## Large language models for material property predictions: elastic constant tensor prediction and materials design

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A multifunctional LLM for predicting finite temperature elastic constant tensor, RAG-enhanced prediction, and inverse material design.

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