

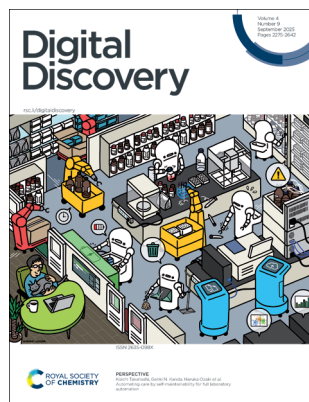
# Digital Discovery

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## IN THIS ISSUE

ISSN 2635-098X CODEN DDIIAI 4(9) 2275–2642 (2025)



### Cover

See Koichi Takahashi, Genki N. Kanda, Haruka Ozaki *et al.*, pp. 2285–2297. Image reproduced by permission of Hiroko Uchida from *Digital Discovery*, 2025, 4, 2285.



### Inside cover

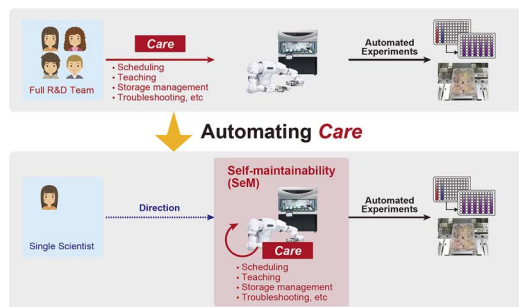
See Rahul Sheshanarayana and Fengqi You, pp. 2298–2335. Image reproduced by permission of Fengqi You from *Digital Discovery*, 2025, 4, 2298.

## PERSPECTIVE

2285

### Automating care by self-maintainability for full laboratory automation

Koji Ochiai, Yuya Tahara-Arai, Akari Kato, Kazunari Kaizu, Hirokazu Kariyazaki, Makoto Umeno, Koichi Takahashi,\* Genki N. Kanda\* and Haruka Ozaki\*

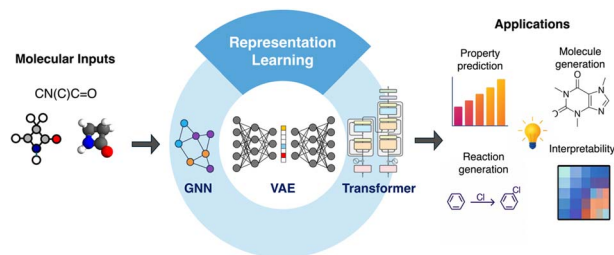


## REVIEWS

2298

### Molecular representation learning: cross-domain foundations and future Frontiers

Rahul Sheshanarayana and Fengqi You\*



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# EES Solar

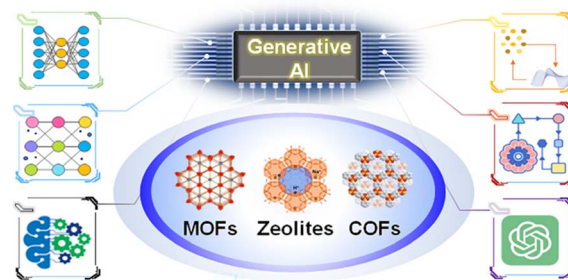
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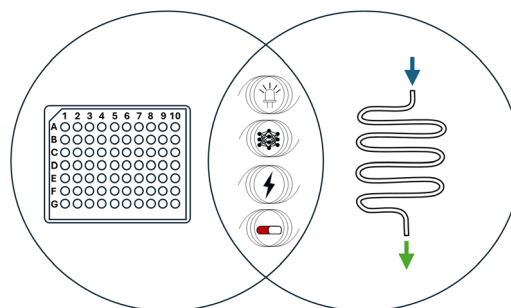
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## REVIEWS

2336

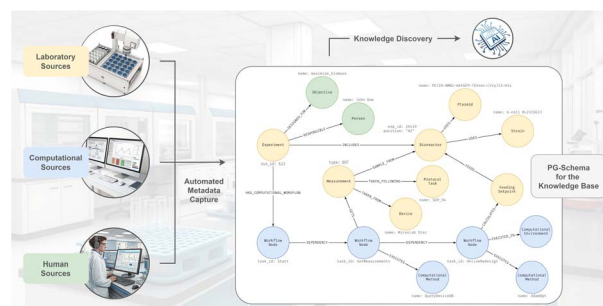
**Generative AI for design of nanoporous materials: review and future prospects**Evan Xie, Xijun Wang,<sup>\*</sup> J. Ilja Siepmann, Haoyuan Chen and Randall Q. Snurr<sup>\*</sup>

2364

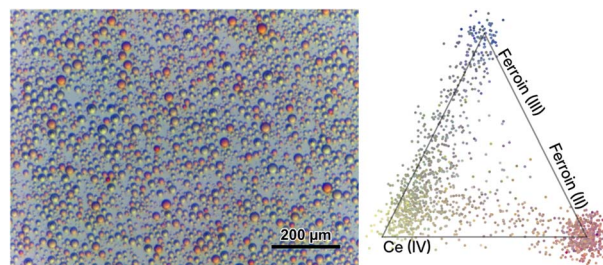
**Flow chemistry as a tool for high throughput experimentation**George Lyall-Brookes, Alex C. Padgham and Anna G. Slater<sup>\*</sup>

## PAPERS

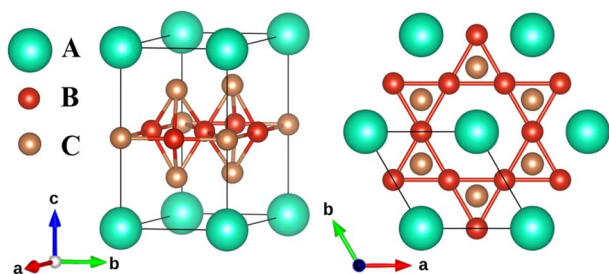
2401

**A property graph schema for automated metadata capture, reproducibility and knowledge discovery in high-throughput bioprocess development**Federico M. Mione, Martin F. Luna, Lucas Kasperetz, Peter Neubauer, Ernesto C. Martinez and M. Nicolas Cruz Bournazou<sup>\*</sup>

2423

**Programmable aerosol chemistry coupled to chemical imaging establishes a new arena for automated chemical synthesis and discovery**Jakub D. Wosik, Chaoyi Zhu, Zehua Li and S. Hessam M. Mehr<sup>\*</sup>

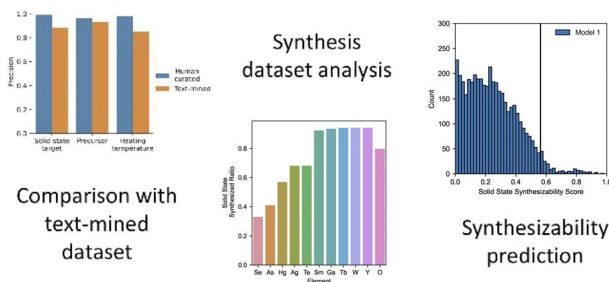
2431



### High-throughput study of kagome compounds in the $AV_3Sb_5$ family

Thalis H. B. da Silva, Tiago F. T. Cerqueira, Hai-Chen Wang and Miguel A. L. Marques\*

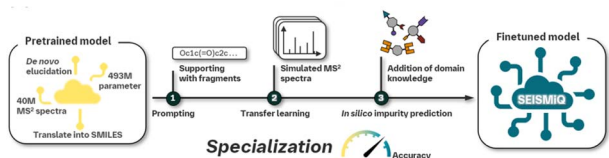
2439



### Solid-state synthesizability predictions using positive-unlabeled learning from human-curated literature data

Vincent Chung,\* Aron Walsh and David J. Payne

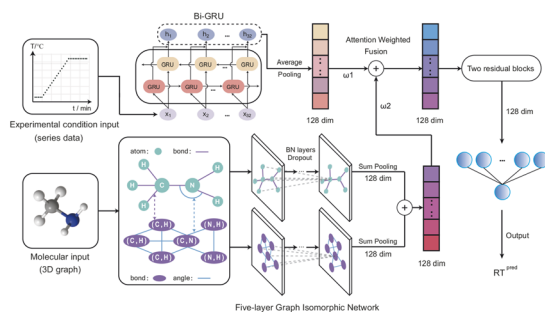
2454



### Enhancing automated drug substance impurity structure elucidation from tandem mass spectra through transfer learning and domain knowledge

Emilio Dorigatti, Jonathan Groß, Jonas Kühlborn, Robert Möckel, Frank Maier\* and Julian Keupp\*

2465



### Multimodal learning in synthetic chemistry applications: gas chromatography retention time prediction and isomer separation optimization

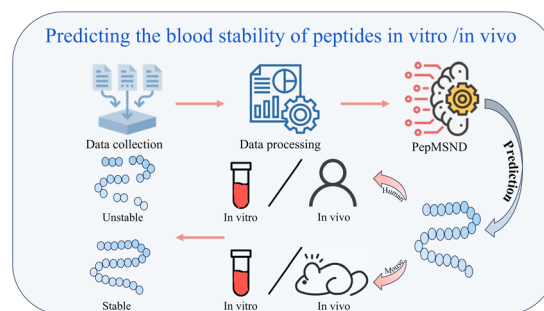
Jinglong Lin, Longyin Song, Yuntian Chen, Chengchun Liu, Shufeng Chen\* and Fanyang Mo\*



2478

## PepMSND: integrating multi-level feature engineering and comprehensive databases to enhance *in vitro/in vivo* peptide blood stability prediction

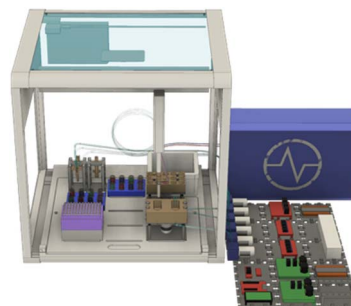
Haomeng Hu, Chengyun Zhang, Zhenyu Xu, Jingjing Guo, An Su, Chengxi Li and Hongliang Duan\*



2491

## AMPERE-2: an open-hardware, robotic platform for automated electrodeposition and electrochemical validation

Nis Fisker-Bødker,\* Daniel Persaud, Yang Bai,\* Mark Kozdras, Tejs Vegge, Jason Hattrick-Simpers and Jin Hyun Chang\*

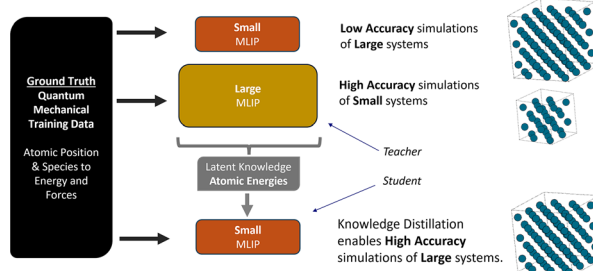


2502

## Teacher-student training improves the accuracy and efficiency of machine learning interatomic potentials

Sakib Matin,\* Alice E. A. Allen, Emily Shinkle, Aleksandra Pachaliewa, Galen T. Craven, Benjamin Nebgen, Justin S. Smith, Richard Messerly, Ying Wai Li, Sergei Tretiak, Kipton Barros and Nicholas Lubbers

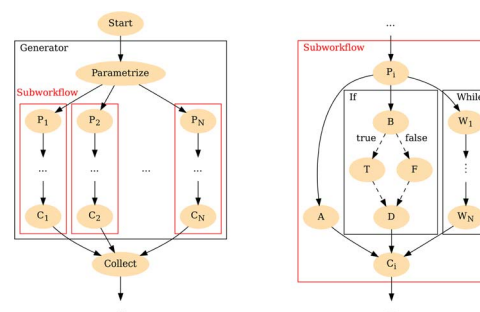
### Knowledge Distillation for Machine Learning Interatomic potentials (MLIPs)



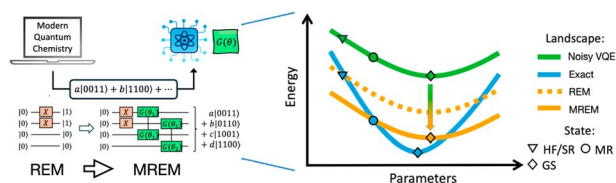
2512

## Taskblaster: a generic framework for automated computational workflows

Ask Hjorth Larsen,\* Mikael J. Kuisma,\* Tara M. Boland, Fredrik A. Nilsson and Kristian S. Thygesen



2521

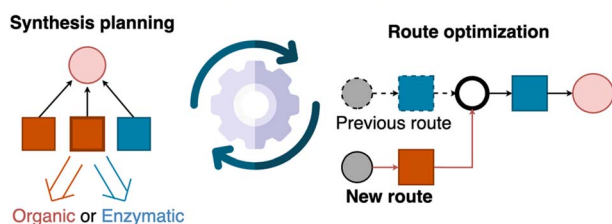


### Multireference error mitigation for quantum computation of chemistry

Hang Zou, Erika Magnusson, Hampus Brunander, Werner Dobrautz\* and Martin Rahm

2534

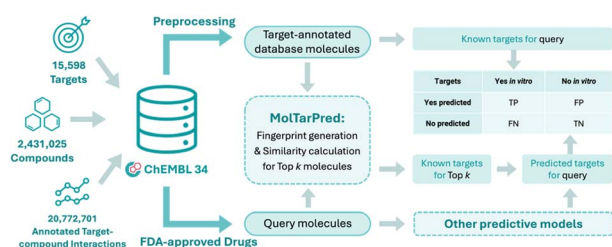
### Synthetic potential in chemoenzymatic retrosynthesis



### Chemoenzymatic synthesis planning guided by synthetic potential scores

Xuan Liu, Hongxiang Li and Huimin Zhao\*

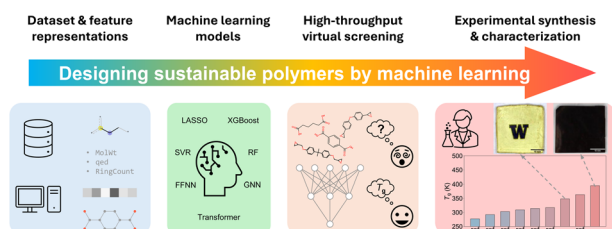
2548



### A precise comparison of molecular target prediction methods

Tiantian He, Klaudia Caba and Pedro J. Ballester\*

2559



### Toward sustainable polymer design: a molecular dynamics-informed machine learning approach for vitrimers

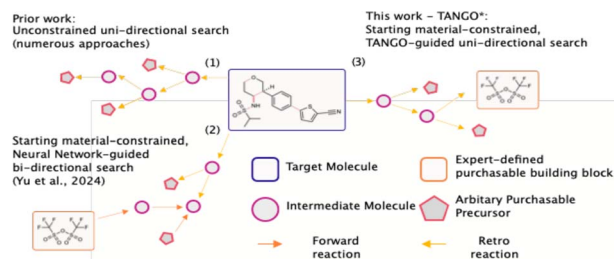
Yiwen Zheng, Agni K. Biswal, Yaqi Guo, Prakash Thakolkaran, Yash Kokane, Vikas Varshney, Siddhant Kumar and Aniruddh Vashisth\*



2570

## Tango\*: constrained synthesis planning using chemically informed value functions

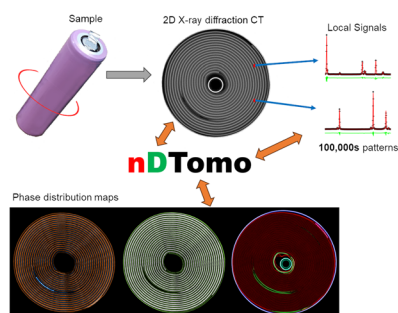
Daniel Armstrong,\* Zlatko Jončev, Jeff Guo and Philippe Schwaller\*



2579

## nDTomo: a modular Python toolkit for X-ray chemical imaging and tomography

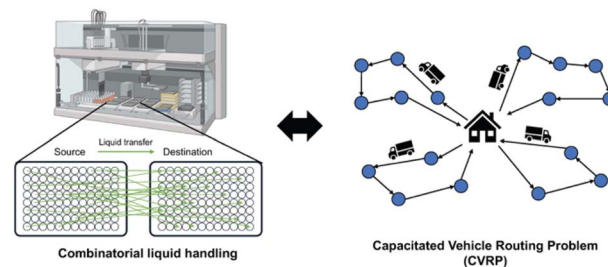
A. Vamvakeros,\* E. Papoutsellis, H. Dong, R. Docherty, A. M. Beale, S. J. Cooper and S. D. M. Jacques



2593

## Optimization of robotic liquid handling as a capacitated vehicle routing problem

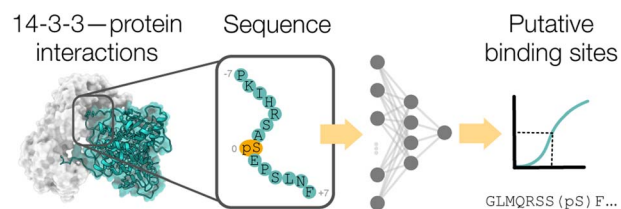
Guangqi Wu, Runzhong Wang and Connor. W. Coley\*



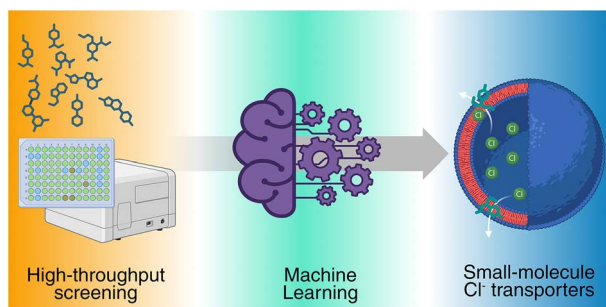
2602

## Identifying 14-3-3 interactome binding sites with deep learning

Laura van Weesep, Rıza Özçelik, Marloes Pennings, Emanuele Criscuolo, Christian Ottmann, Luc Brunsveld\* and Francesca Grisoni\*



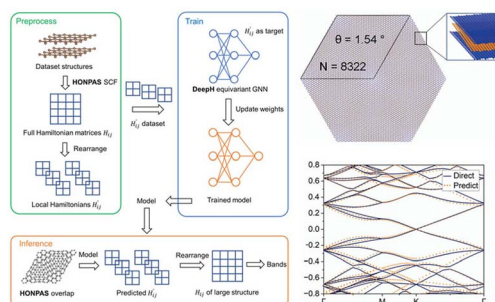
2615



### Development of synthetic chloride transporters using high-throughput screening and machine learning

Surid Mohammad Chowdhury, Nada J. Daood, Katherine R. Lewis, Rayhanus Salam, Hao Zhu\* and Nathalie Busschaert\*

2627



### Combining DeepH with HONPAS for accurate and efficient hybrid functional electronic structure calculations with ten thousand atoms

Yifan Ke, Xinming Qin,\* Wei Hu\* and Jinlong Yang\*

## CORRECTION

2639

### Correction: Atomate2: modular workflows for materials science

Alex M. Ganose,\* Hrushikesh Sahasrabuddhe, Mark Asta, Kevin Beck, Tathagata Biswas, Alexander Bonkowski, Joana Bustamante, Xin Chen, Yuan Chiang, Daryl C. Chrzan, Jacob Clary, Orion A. Cohen, Christina Ertural, Max C. Gallant, Janine George, Sophie Gerits, Rhys E. A. Goodall, Rishabh D. Guha, Geoffroy Hautier, Matthew Horton, T. J. Inizan, Aaron D. Kaplan, Ryan S. Kingsbury, Matthew C. Kuner, Bryant Li, Xavier Linn, Matthew J. McDermott, Rohith Srinivaas Mohanakrishnan, Aakash A. Naik, Jeffrey B. Neaton, Shehan M. Parmar, Kristin A. Persson, Guido Petretto, Thomas A. R. Purcell, Francesco Ricci, Benjamin Rich, Janosh Riebesell, Gian-Marco Rignanese, Andrew S. Rosen, Matthias Scheffler, Jonathan Schmidt, Jimmy-Xuan Shen, Andrei Sobolev, Ravishankar Sundararaman, Cooper Tezak, Victor Trinquet, Joel B. Varley, Derek Vigil-Fowler, Duo Wang, David Waroquiers, Mingjian Wen, Han Yang, Hui Zheng, Jiongzhi Zheng, Zhuoying Zhu and Anubhav Jain\*

