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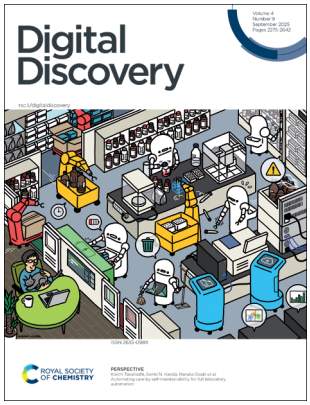

Cover
See Koichi Takahashi, Genki N. Kanda, Haruka Ozaki *et al.*, pp. 2285–2297. Image reproduced by permission of Hiroko Uchida from *Digital Discovery*, 2025, **4**, 2285.

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

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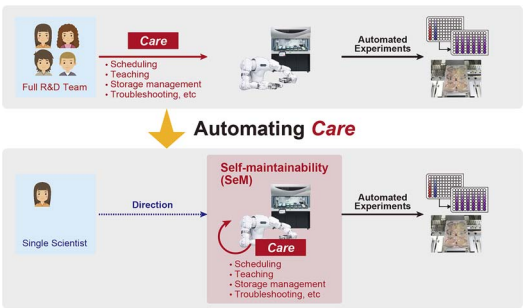
Automating *care* by self-maintainability for full laboratory automation

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



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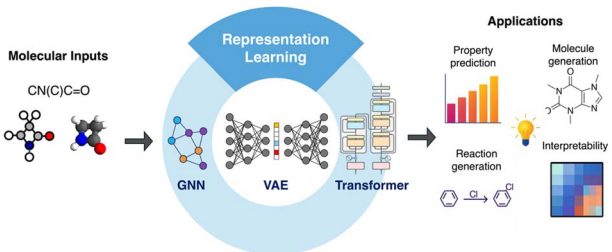
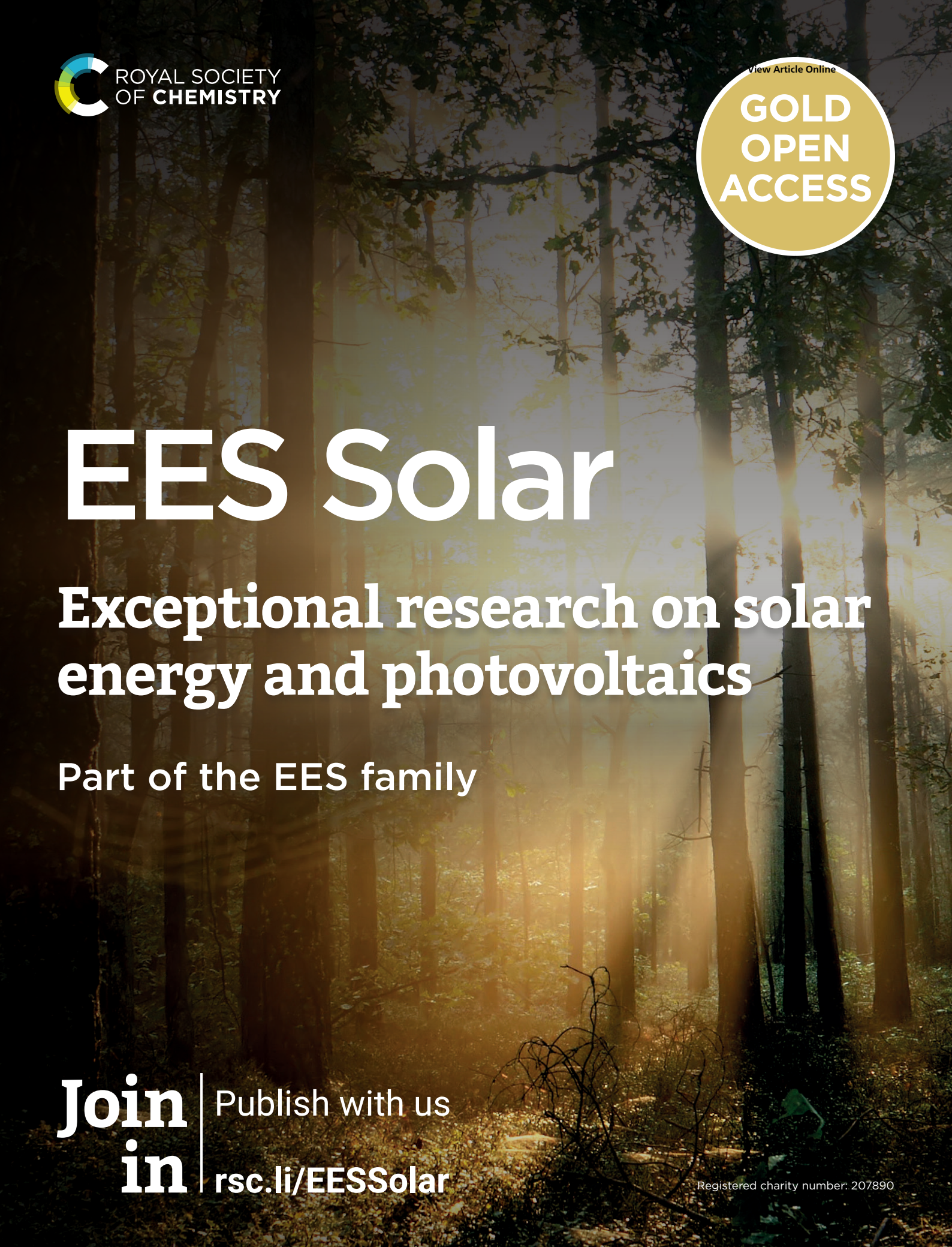
Molecular representation learning: cross-domain foundations and future Frontiers

Rahul Sheshanarayana and Fengqi You*

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REVIEWS

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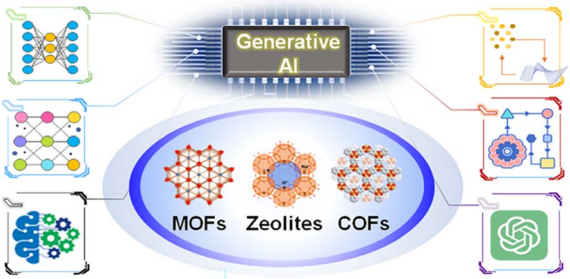
Generative AI for design of nanoporous materials: review and future prospects

Evan Xie, Xijun Wang,* J. Ilja Siepmann, Haoyuan Chen and Randall Q. Snurr*



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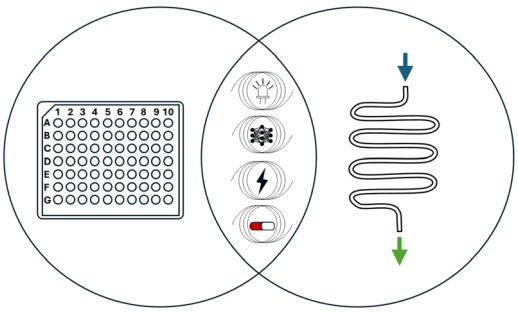
Flow chemistry as a tool for high throughput experimentation

George Lyall-Brookes, Alex C. Padgham and Anna G. Slater*



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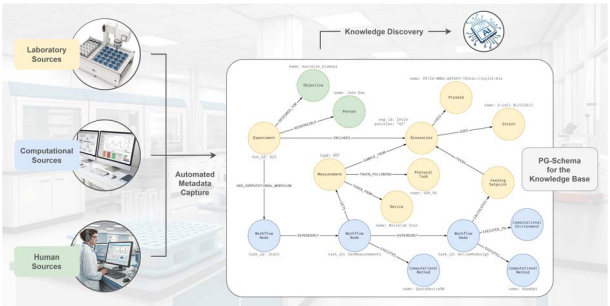
A property graph schema for automated metadata capture, reproducibility and knowledge discovery in high-throughput bioprocess development

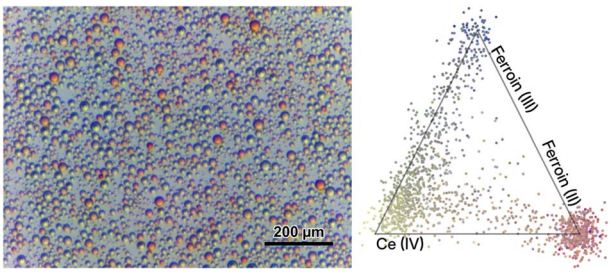
Federico M. Mione, Martin F. Luna, Lucas Kaspersetz, Peter Neubauer, Ernesto C. Martinez and M. Nicolas Cruz Bournazou*



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*



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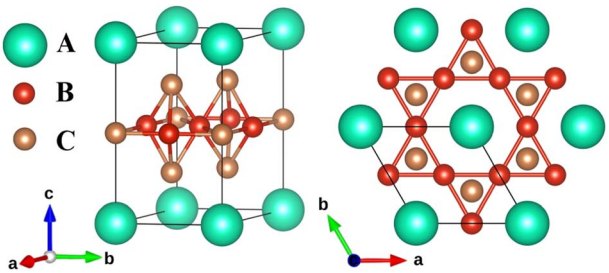

High-throughput study of kagome compounds in the AV_3Sb_5 family

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

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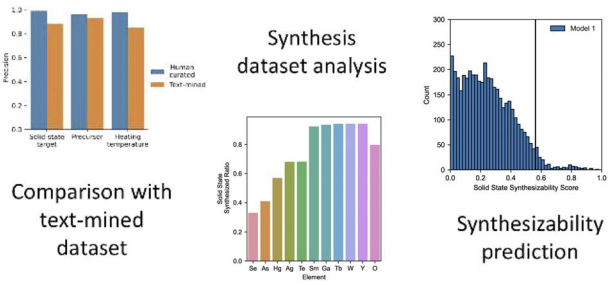

Solid-state synthesizability predictions using positive-unlabeled learning from human-curated literature data

Vincent Chung,* Aron Walsh and David J. Payne

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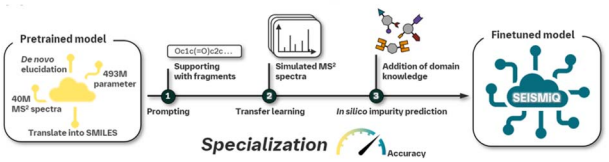

Enhancing automated drug substance impurity structure elucidation from tandem mass spectra through transfer learning and domain knowledge

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

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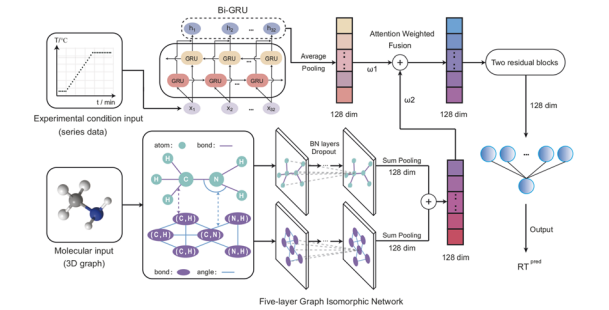

Multimodal learning in synthetic chemistry applications: gas chromatography retention time prediction and isomer separation optimization

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

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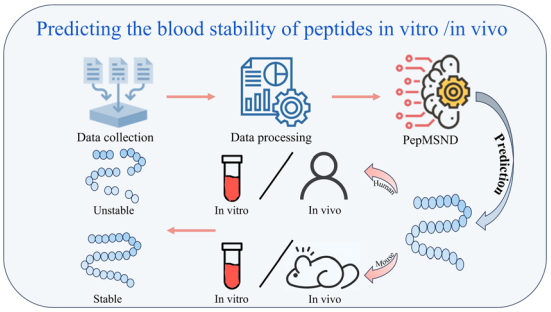
PepMSND: integrating multi-level feature engineering and comprehensive databases to enhance *in vitro*/*in vivo* peptide blood stability prediction

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



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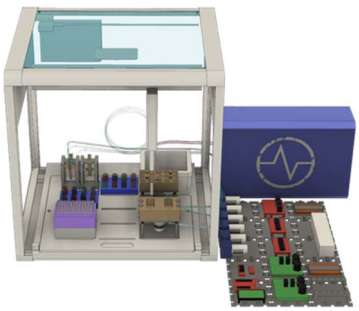
AMPERE-2: an open-hardware, robotic platform for automated electrodeposition and electrochemical validation

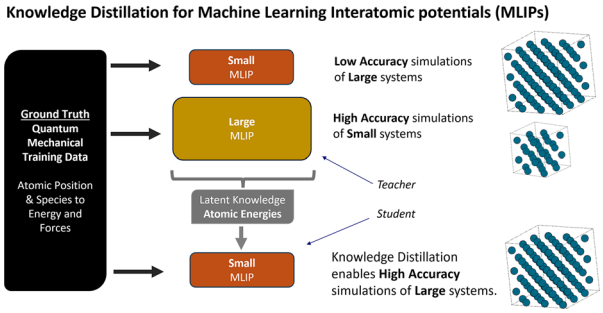
Nis Fisker-Bødker,* Daniel Persaud, Yang Bai,* Mark Kozdras, Tejs Vegge, Jason Hattrick-Simpers and Jin Hyun Chang*



2502

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

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



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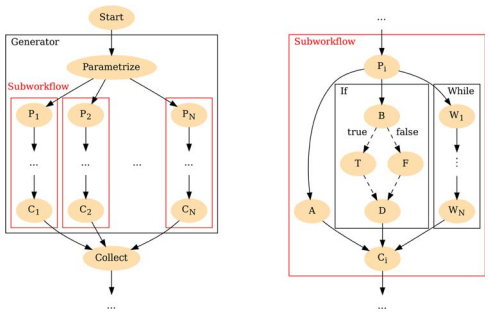
Taskblaster: a generic framework for automated computational workflows

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



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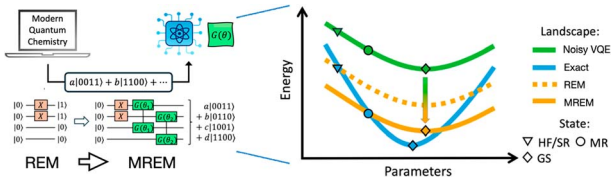

Multireference error mitigation for quantum computation of chemistry

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

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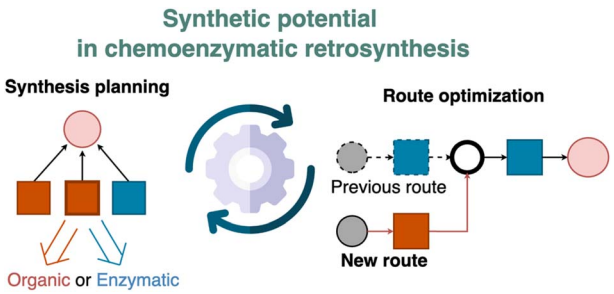

Chemoenzymatic synthesis planning guided by synthetic potential scores

Xuan Liu, Hongxiang Li and Huimin Zhao*

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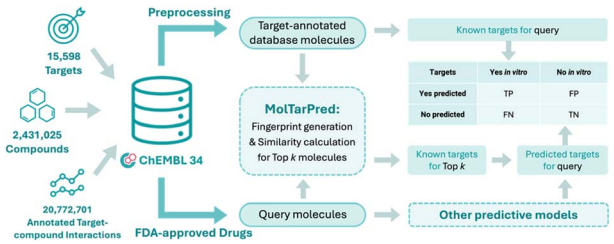

A precise comparison of molecular target prediction methods

Tiantian He, Klaudia Caba and Pedro J. Ballester*

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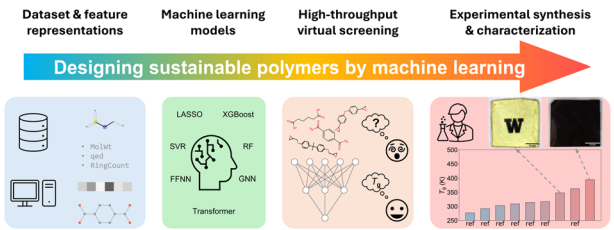

Toward sustainable polymer design: a molecular dynamics-informed machine learning approach for vitrimers

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

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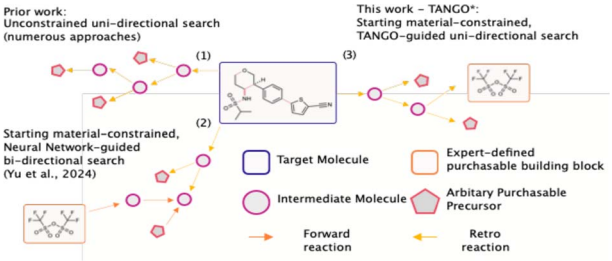
Tango*: constrained synthesis planning using chemically informed value functions

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



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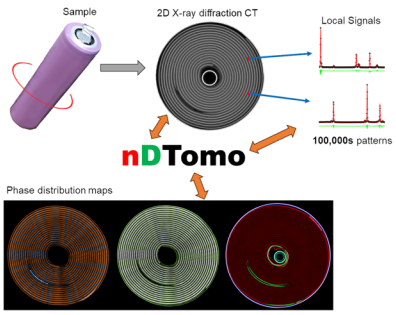
***nDTomo*: a modular Python toolkit for X-ray chemical imaging and tomography**

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



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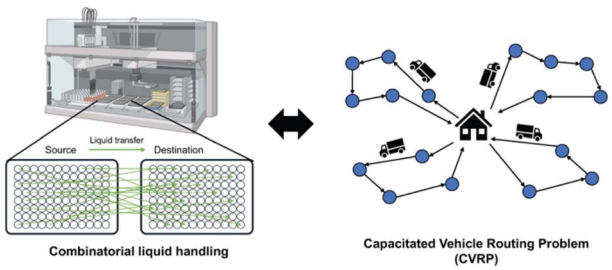
Optimization of robotic liquid handling as a capacitated vehicle routing problem

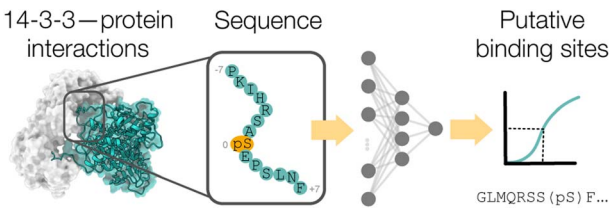
Guangqi Wu, Runzhong Wang and Connor. W. Coley*



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*



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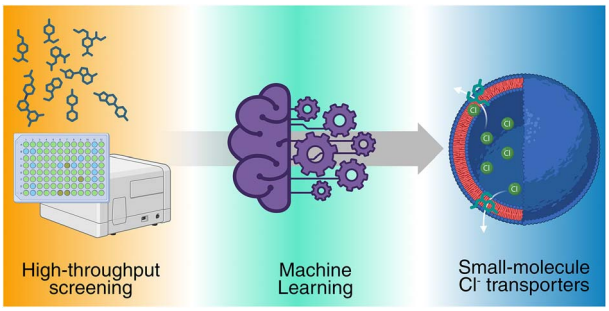

Development of synthetic chloride transporters using high-throughput screening and machine learning

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

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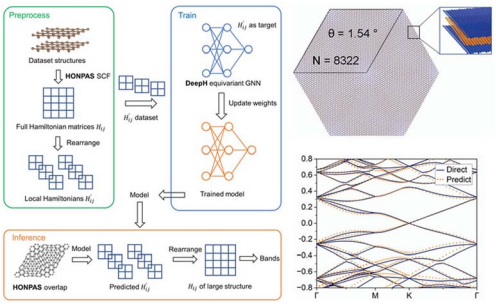

Combining DeepH with HONPAS for accurate and efficient hybrid functional electronic structure calculations with ten thousand atoms

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

CORRECTION

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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*

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