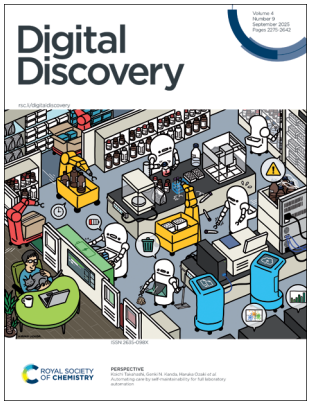
Digital Discovery

rsc.li/digitaldiscovery

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

IN THIS ISSUE

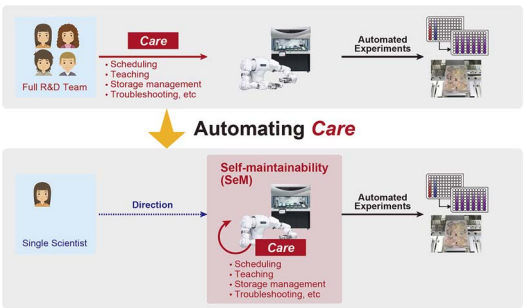
ISSN 2635-098X CODEN DDIIAI 4(9) 2275–2642 (2025)



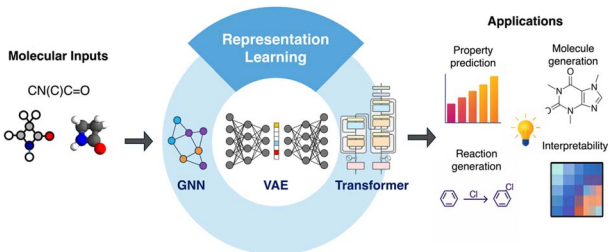
Cover
See Koichi Takahashi, Genki N. Kanda, Haruka Ozaki *et al.*, pp. 2285–2297. Image reproduced by permission of Hiroko Uchida from *Digital Discovery*, 2025, **4**, 2285.

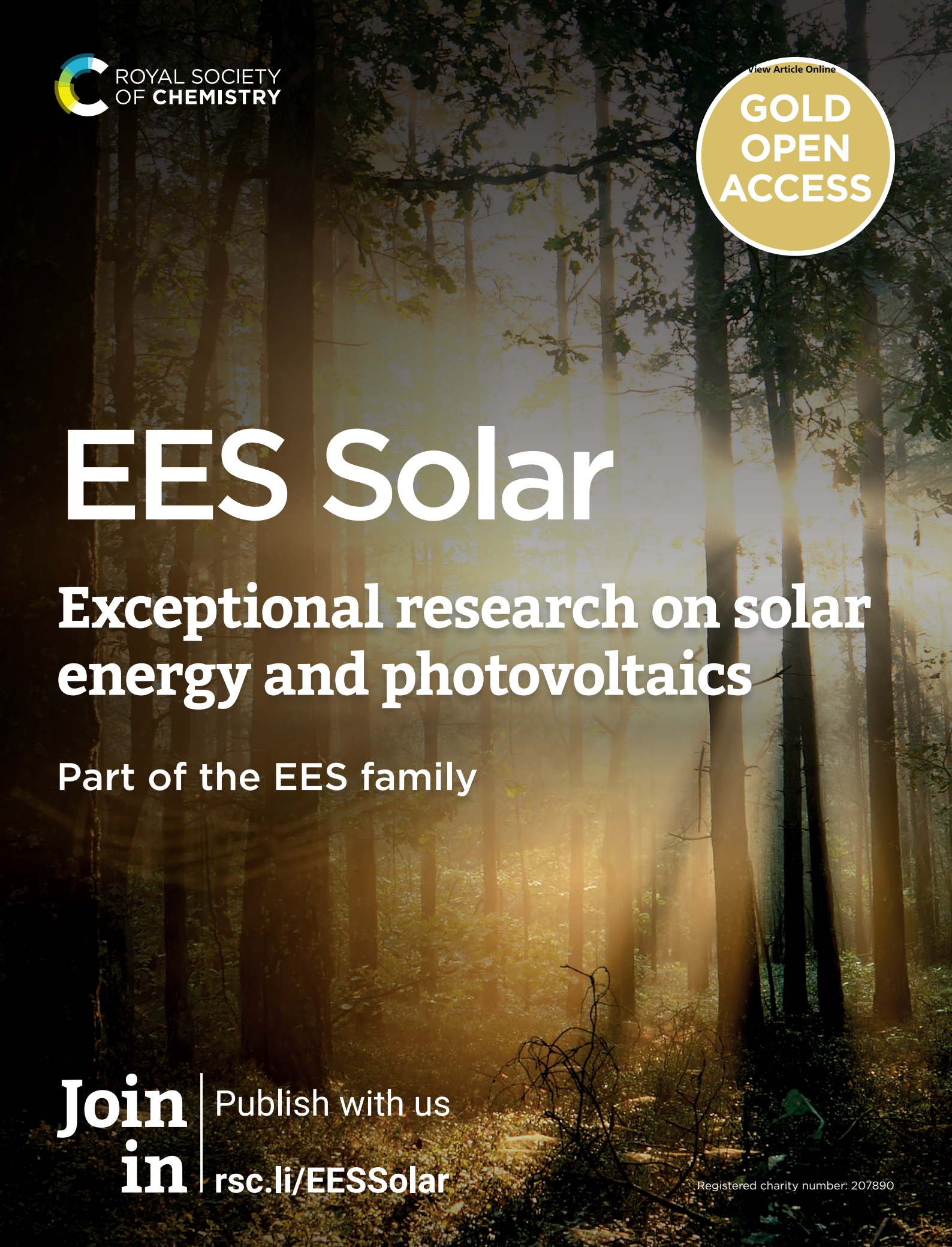
Inside cover
See Rahul Sheshanarayana and Fengqi You, pp. 2298–2335. Image reproduced by permission of Fengqi You from *Digital Discovery*, 2025, **4**, 2298.

PERSPECTIVE

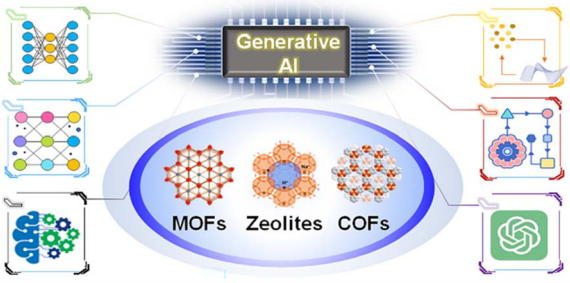


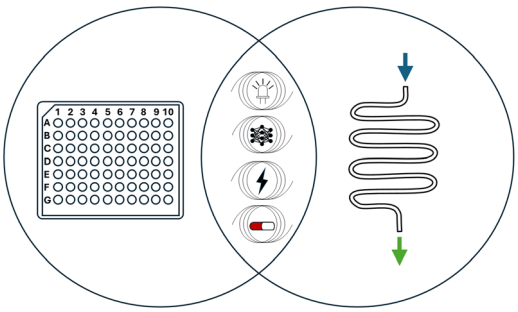
REVIEWS



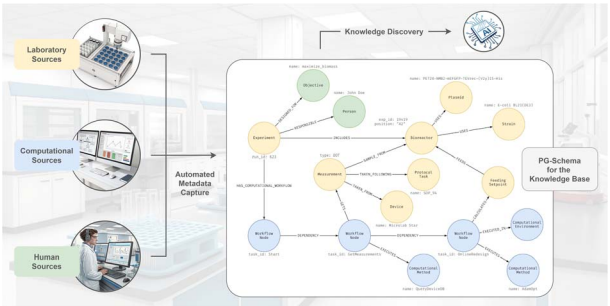

ROYAL SOCIETY OF CHEMISTRY
View Article Online
GOLD OPEN ACCESS
EES Solar
Exceptional research on solar energy and photovoltaics
Part of the EES family
Join in
Publish with us
rsc.li/EESSolar
Registered charity number: 207890

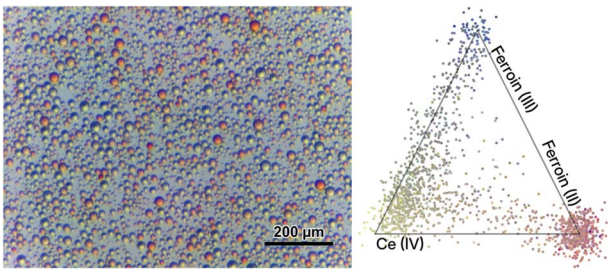
REVIEWS





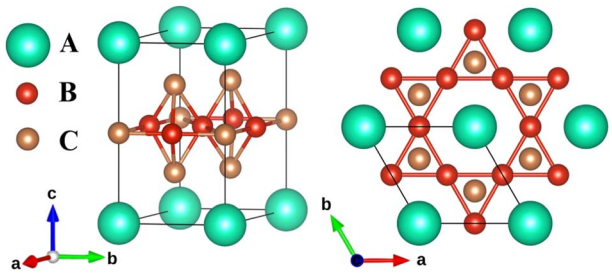
PAPERS





PAPERS

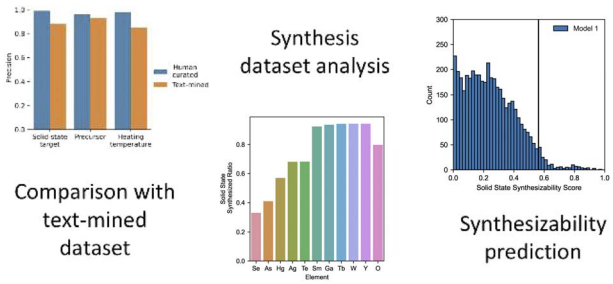
2431



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*

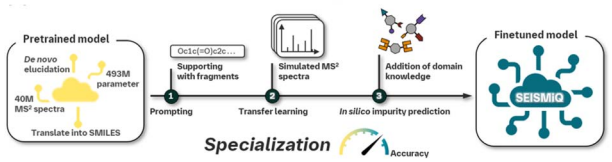
2439



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

Vincent Chung,* Aron Walsh and David J. Payne

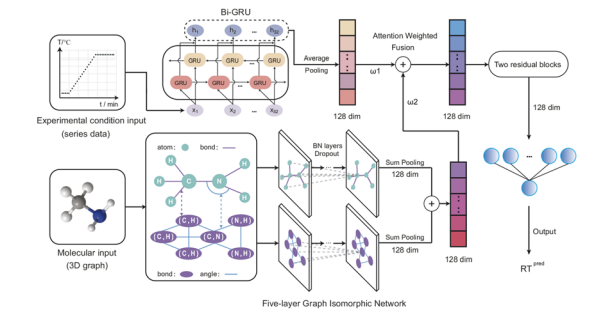
2454



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*

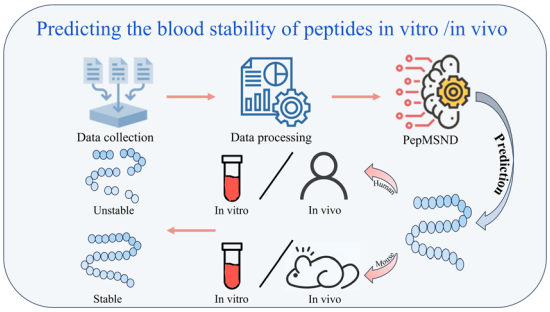
2465

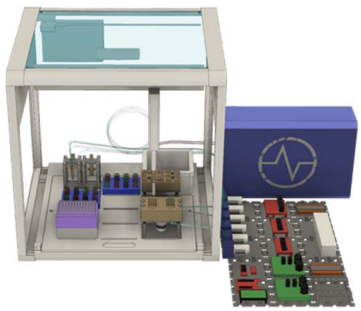


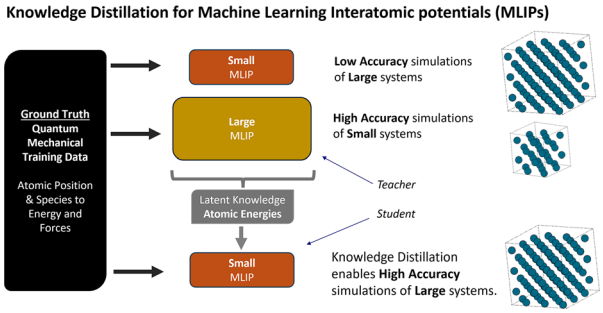
Multimodal learning in synthetic chemistry applications: gas chromatography retention time prediction and isomer separation optimization

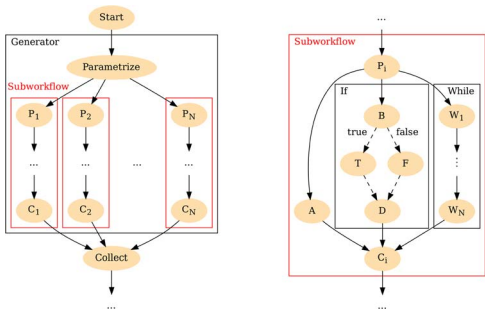
Jinglong Lin, Longyin Song, Yuntian Chen, Chengchun Liu, Shufeng Chen* and Fanyang Mo*

PAPERS









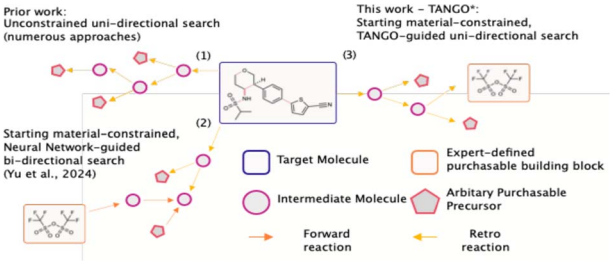
PAPERS

PAPERS

2570

Tango*: constrained synthesis planning using chemically informed value functions

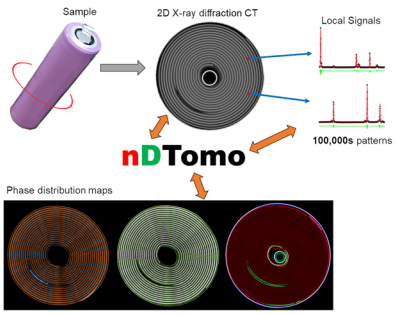
Daniel Armstrong,* Zlatko Jončev, Jeff Guo and Philippe Schwaller*



2579

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

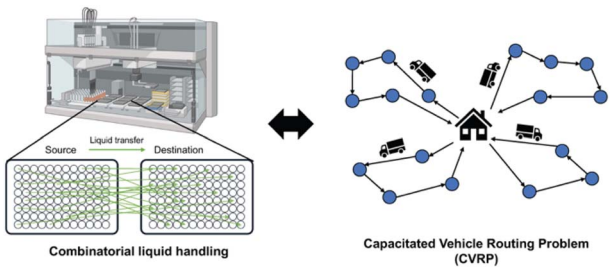
A. Vamvakeros,* E. Papoutsellis, H. Dong, R. Docherty, A. M. Beale, S. J. Cooper and S. D. M. Jacques



2593

Optimization of robotic liquid handling as a capacitated vehicle routing problem

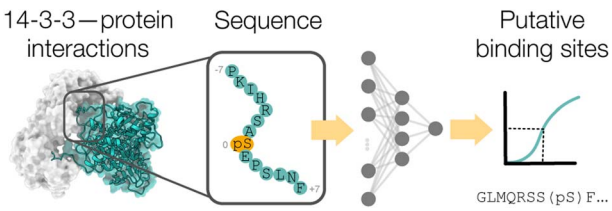
Guangqi Wu, Runzhong Wang and Connor. W. Coley*



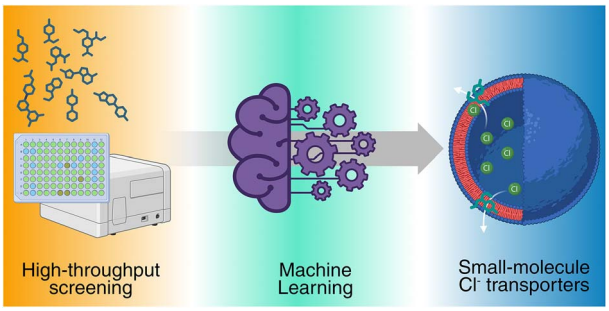
2602

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*

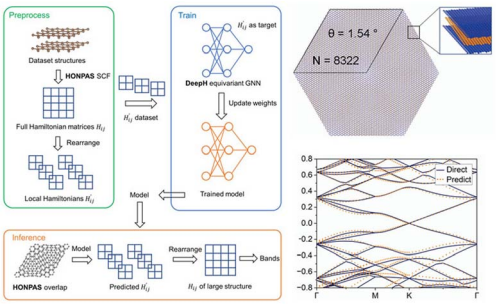


PAPERS



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*



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

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*