

# 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.

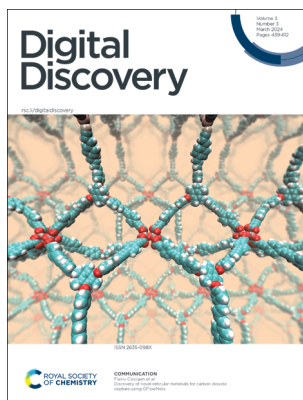
## IN THIS ISSUE

ISSN 2635-098X CODEN DDIIAI 3(3) 439–612 (2024)



### Cover

See Rama K. Vasudevan *et al.*, pp. 456–466. Image reproduced by permission of Andrew Sproles (artist), Oak Ridge National Laboratory (ORNL) from *Digital Discovery*, 2024, 3, 456.



### Inside cover

See Flaviu Cipcigan *et al.*, pp. 449–455. Image reproduced by permission of Flaviu Cipcigan from *Digital Discovery*, 2024, 3, 449.

## EDITORIAL

447

### Guidelines for hardware-focused articles

Jason E. Hein\* and Joshua Schrier\*



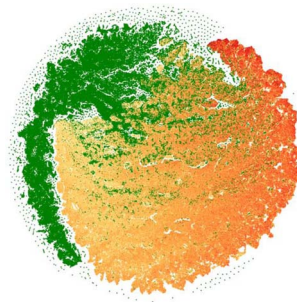
Digital  
Discovery

## COMMUNICATION

449

### Discovery of novel reticular materials for carbon dioxide capture using GFlowNets

Flaviu Cipcigan,\* Jonathan Booth, Rodrigo Neumann Barros Ferreira, Carine Ribeiro dos Santos and Mathias Steiner



# Advance your career in science

with professional recognition that showcases  
your **experience, expertise and dedication**

## Stand out from the crowd

Prove your commitment  
to attaining excellence in  
your field

## Gain the recognition you deserve

Achieve a professional  
qualification that inspires  
confidence and trust

## Unlock your career potential

Apply for our professional  
registers (RSci, RSciTech)  
or chartered status  
(CChem, CSci, CEnv)

## Apply now

[rsc.li/professional-development](https://rsc.li/professional-development)

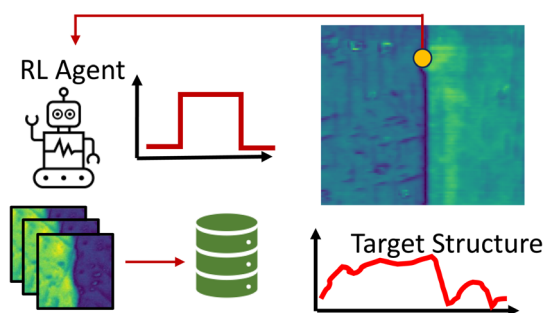


## PAPERS

456

### Physics-informed models of domain wall dynamics as a route for autonomous domain wall design via reinforcement learning

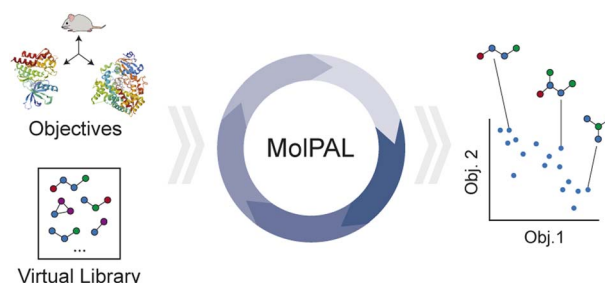
Benjamin R. Smith, Bharat Pant, Yongtao Liu, Yu-Chen Liu, Jan-Chi Yang, Stephen Jesse, Anahita Khojandi, Sergei V. Kalinin, Ye Cao and Rama K. Vasudevan\*



467

### Pareto optimization to accelerate multi-objective virtual screening

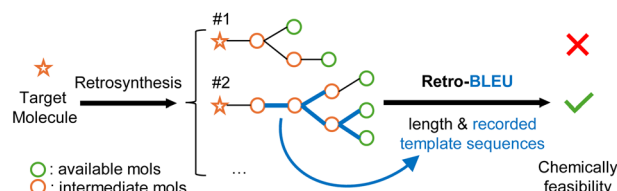
Jenna C. Fromer, David E. Graff and Connor W. Coley\*



482

### Retro-BLEU: quantifying chemical plausibility of retrosynthesis routes through reaction template sequence analysis

Junren Li, Lei Fang\* and Jian-Guang Lou



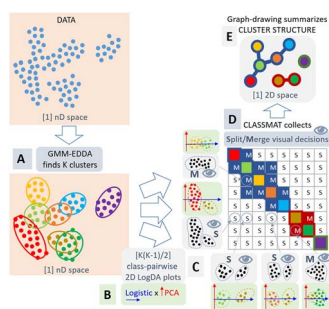
491

### Image and data mining in reticular chemistry powered by GPT-4V

Zhiling Zheng, Zhiguo He, Omar Khattab, Nakul Rampal, Matei A. Zaharia, Christian Borgs, Jennifer T. Chayes and Omar M. Yaghi\*



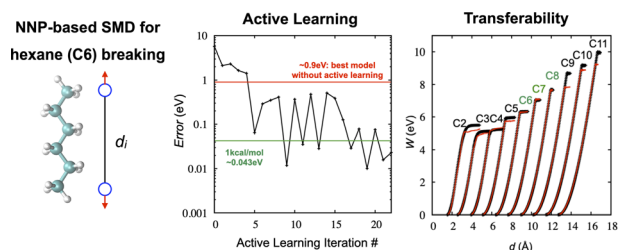
502



## A human-in-the-loop approach for visual clustering of overlapping materials science data

Satyanarayana Bonakala, Michael Aupetit, Halima Bensmail and Fedwa El-Mellouhi\*

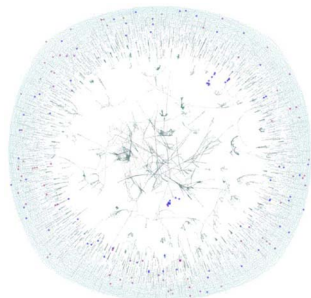
514



## Active learning of neural network potentials for rare events

Gang Seob Jung,\* Jong Youl Choi and Sangkeun Matthew Lee

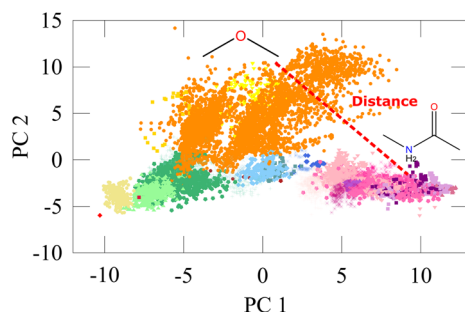
528



## Chemical space analysis and property prediction for carbon capture solvent molecules

James L. McDonagh,\* Stamatia Zavitsanou, Alexander Harrison, Dmitry Zubarev, Theodore van Kessel, Benjamin H. Wunsch and Flaviu Cipcigan\*

544



## Global geometry of chemical graph neural network representations in terms of chemical moieties

Amer Marwan El-Samman,\* Incé Amina Husain, Mai Huynh, Stefano De Castro, Brooke Morton and Stijn De Baerdemacker

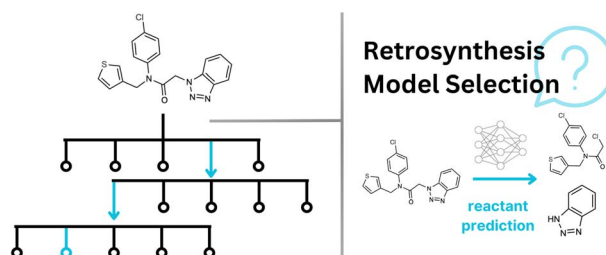


## PAPERS

558

**Models Matter: the impact of single-step retrosynthesis on synthesis planning**

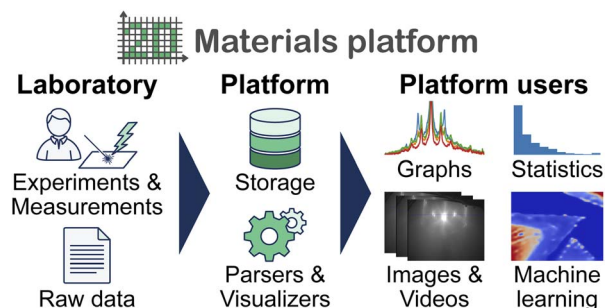
Paula Torren-Peraire,<sup>\*</sup> Alan Kai Hassen,<sup>\*</sup> Samuel Genheden, Jonas Verhoeven, Djork-Arné Clevert, Mike Preuss and Igor V. Tetko



573

**<https://2DMat.ChemDX.org>: Experimental data platform for 2D materials from synthesis to physical properties**

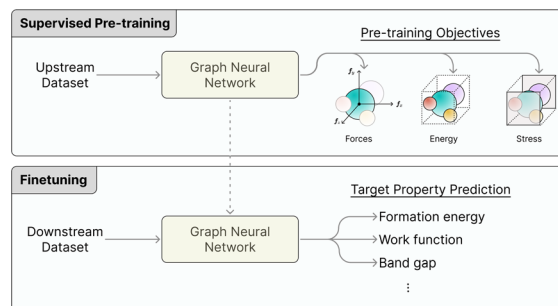
Jin-Hoon Yang, Habin Kang, Hyuk Jin Kim, Taeho Kim, Heonsu Ahn, Tae Gyu Rhee, Yeong Gwang Khim, Byoung Ki Choi, Moon-Ho Jo, Hyunju Chang, Jonghwan Kim,<sup>\*</sup> Young Jun Chang<sup>\*</sup> and Yea-Lee Lee<sup>\*</sup>



586

**Derivative-based pre-training of graph neural networks for materials property predictions**

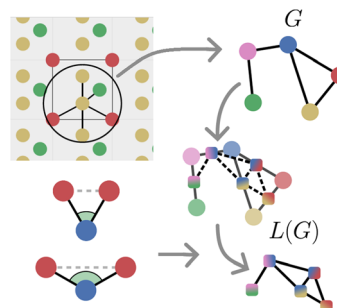
Shuyi Jia, Akaash R. Parthasarathy, Rui Feng, Guojing Cong, Chao Zhang and Victor Fung<sup>\*</sup>



594

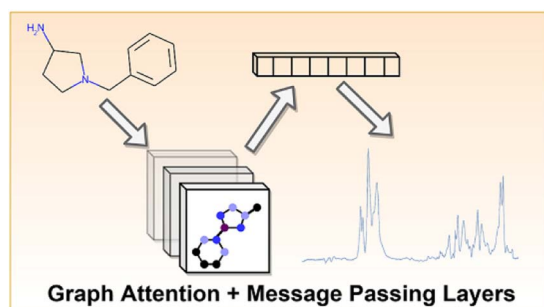
**Connectivity optimized nested line graph networks for crystal structures**

Robin Ruff, Patrick Reiser, Jan Stühmer and Pascal Friederich<sup>\*</sup>



## PAPERS

602

**Infrared spectra prediction using attention-based graph neural networks**

Naseem Saquer, Razib Iqbal,<sup>\*</sup> Joshua D. Ellis and Keiichi Yoshimatsu<sup>\*</sup>

## CORRECTION

610

**Correction: Understanding the patterns that neural networks learn from chemical spectra**

Laura Hannemose Rieger, Max Wilson, Tejs Vegge and Eibar Flores<sup>\*</sup>

