

# 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 DDIAI 3(5) 833–1072 (2024)



**Cover**  
See Stanley Lo, Sterling G. Baird, Taylor D. Sparks, Alán Aspuru-Guzik *et al.*, pp. 842–868.  
Icon made by Freepik, VectorPortal from [www.flaticon.com](http://www.flaticon.com). Image reproduced by permission of Stanley Lo, Alán Aspuru-Guzik and Helen Tran from *Digital Discovery*, 2024, 3, 842.



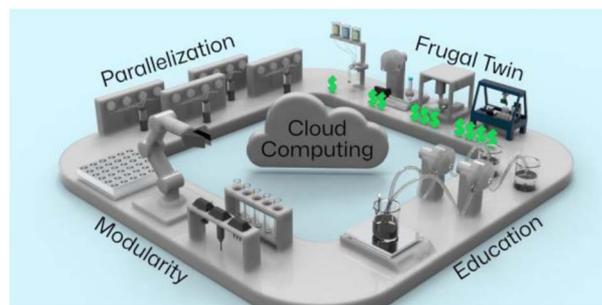
**Inside cover**  
See Mingjian Wen *et al.*, pp. 869–882. Image reproduced by permission of Mingjian Wen from *Digital Discovery*, 2024, 3, 869.

## TUTORIAL REVIEW

842

### Review of low-cost self-driving laboratories in chemistry and materials science: the “frugal twin” concept

Stanley Lo,\* Sterling G. Baird,\* Joshua Schrier, Ben Blaiszik, Nessa Carson, Ian Foster, Andrés Aguilar-Granda, Sergei V. Kalinin, Benji Maruyama, Maria Politi, Helen Tran, Taylor D. Sparks\* and Alán Aspuru-Guzik\*

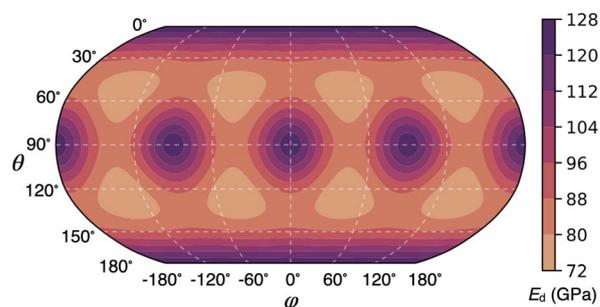


## PAPERS

869

### An equivariant graph neural network for the elasticity tensors of all seven crystal systems

Mingjian Wen,\* Matthew K. Horton, Jason M. Munro, Patrick Huck and Kristin A. Persson



# Royal Society of Chemistry approved training courses

Explore your options.  
Develop your skills.  
Discover learning  
that suits you.

**Courses in the classroom,  
the lab, or online**

Find something for every  
stage of your professional  
development. Search our  
database by:

- subject area
- location
- event type
- skill level

Members **get at least 10% off**

Visit [rsc.li/cpd-training](https://rsc.li/cpd-training)

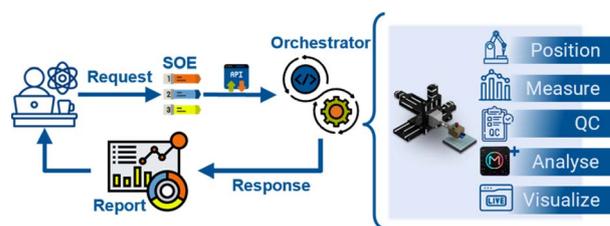


**SAVE  
10%**

883

## Autonomous millimeter scale high throughput battery research system

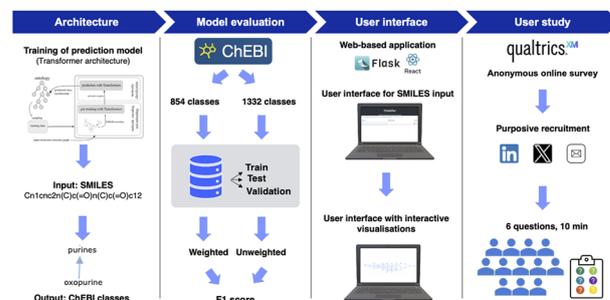
Fuzhan Rahmanian,<sup>\*</sup> Stefan Fuchs, Bojing Zhang, Maximilian Fichtner and Helge Sören Stein<sup>\*</sup>



896

## Chebifier: automating semantic classification in ChEBI to accelerate data-driven discovery

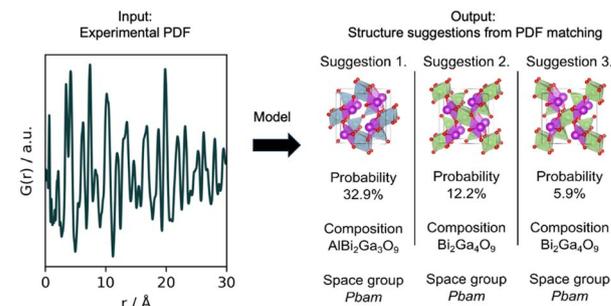
Martin Glauer, Fabian Neuhaus, Simon Flügel, Marie Wosny, Till Mossakowski, Adel Memariani, Johannes Schwerdt and Janna Hastings



908

## MLstructureMining: a machine learning tool for structure identification from X-ray pair distribution functions

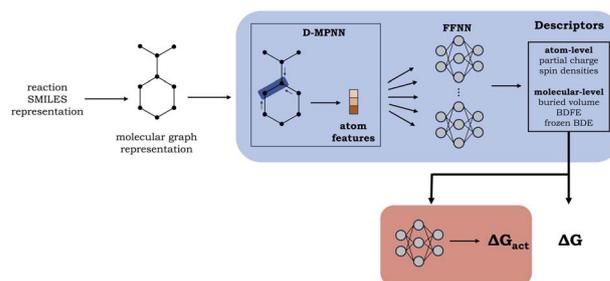
Emil T. S. Kjær, Andy S. Anker, Andrea Kirsch, Joakim Lajer, Olivia Aalling-Frederiksen, Simon J. L. Billinge<sup>\*</sup> and Kirsten M. Ø. Jensen<sup>\*</sup>



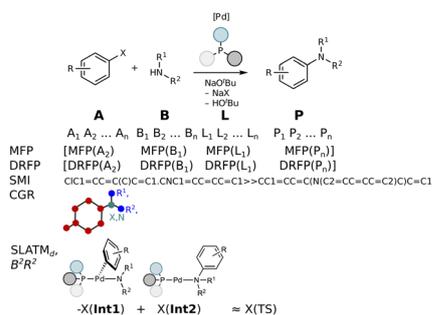
919

## Repurposing quantum chemical descriptor datasets for on-the-fly generation of informative reaction representations: application to hydrogen atom transfer reactions

Javier E. Alfonso-Ramos, Rebecca M. Neeser and Thijs Stuyver<sup>\*</sup>



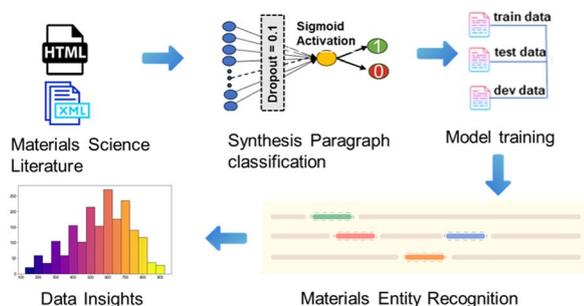
932



## Benchmarking machine-readable vectors of chemical reactions on computed activation barriers

Puck van Gerwen, Ksenia R. Briling, Yannick Calvino Alonso, Malte Franke and Clemence Corminboeuf\*

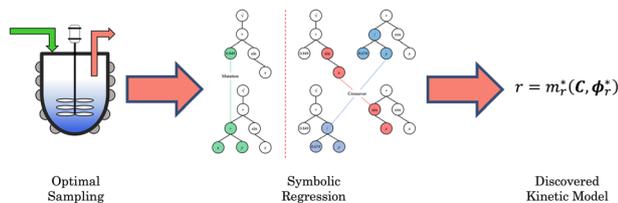
944



## Automated extraction of synthesis parameters of pulsed laser-deposited materials from scientific literature

Rajan Kumar, Ablokot Joshi, Salman A. Khan and Shikhar Misra\*

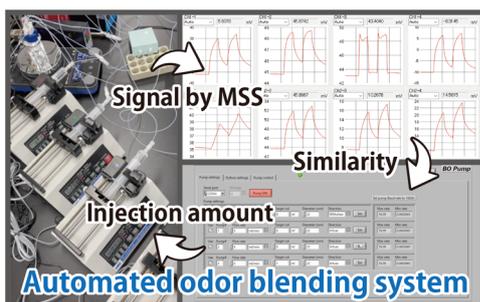
954



## The automated discovery of kinetic rate models – methodological frameworks

Miguel Ángel de Carvalho Servia, Ilya Orson Sandoval, King Kuok (Mimi) Hii, Klaus Hellgardt, Dongda Zhang\* and Ehecatl Antonio del Rio Chanona\*

969



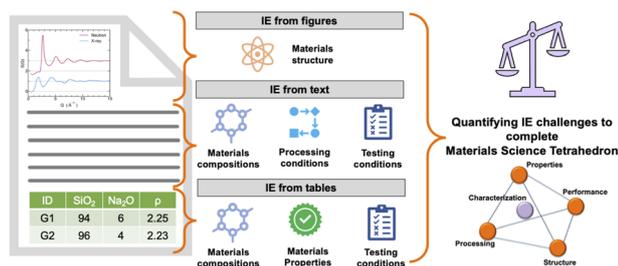
## Automated odor-blending with one-pot Bayesian optimization

Yota Fukui, Kosuke Minami,\* Kota Shiba, Genki Yoshikawa, Koji Tsuda\* and Ryo Tamura\*





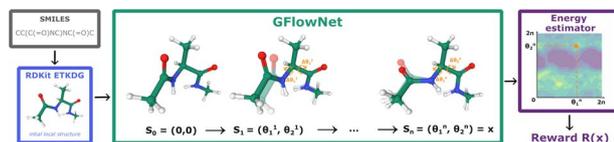
1021



## Reconstructing the materials tetrahedron: challenges in materials information extraction

Kausik Hira, Mohd Zaki, Dhruvil Sheth, Mausam\* and N. M. Anoop Krishnan\*

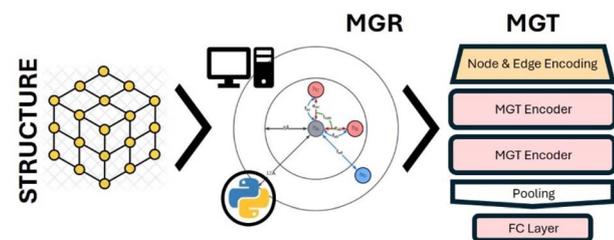
1038



## Towards equilibrium molecular conformation generation with GFlowNets

Alexandra Volokhova,\* Michat Koziarski,\* Alex Hernández-García, Cheng-Hao Liu, Santiago Miret, Pablo Lemos, Luca Thiede, Zichao Yan, Alán Aspuru-Guzik and Yoshua Bengio

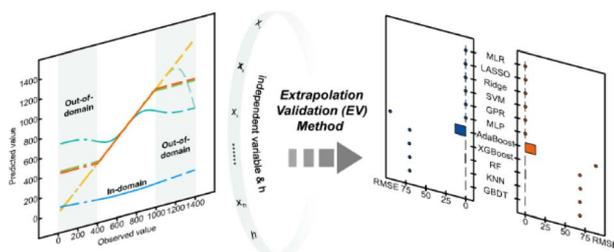
1048



## Molecular graph transformer: stepping beyond ALIGNN into long-range interactions

Marco Anselmi, Greg Slabaugh,\* Rachel Crespo-Otero\* and Devis Di Tommaso\*

1058



## Extrapolation validation (EV): a universal validation method for mitigating machine learning extrapolation risk

Mengxian Yu, Yin-Ning Zhou, Qiang Wang and Fangyou Yan\*



## CORRECTIONS

1068

**Correction: Tackling data scarcity with transfer learning: a case study of thickness characterization from optical spectra of perovskite thin films**

Siyu Isaac Parker Tian, Zekun Ren, Selvaraj Venkataraj, Yuanhang Cheng, Daniil Bash, Felipe Oviedo, J. Senthilnath, Vijila Chellappan, Yee-Fun Lim, Armin G. Aberle, Benjamin P. MacLeod, Fraser G. L. Parlane, Curtis P. Berlinguette, Qianxiao Li, Tonio Buonassisi\* and Zhe Liu\*

1069

**Correction: Predicting small molecules solubility on endpoint devices using deep ensemble neural networks**

Mayk Caldas Ramos and Andrew D. White\*

