

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(12) 2387–2638 (2024)



Cover
See Luokun Zhang and S. Hessam M. Mehr, pp. 2424–2433. Image reproduced by permission of S. Hessam M. Mehr and Luokun Zhang from *Digital Discovery*, 2024, 3, 2424.



Inside cover
See Pascal Miéville *et al.*, pp. 2434–2447. Image reproduced by permission of Pascal Miéville from *Digital Discovery*, 2024, 3, 2434.

REVIEW

2396

Unsupervised learning and pattern recognition in alloy design

Ninad Bhat, Nick Birbilis and Amanda S. Barnard*

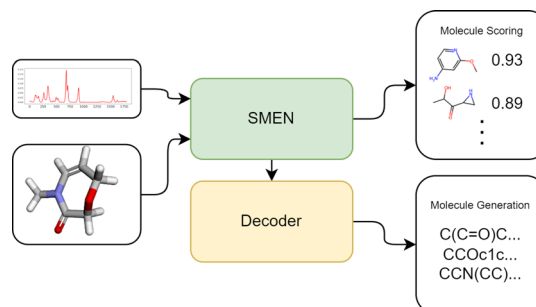


COMMUNICATION

2417

Spectra to structure: contrastive learning framework for library ranking and generating molecular structures for infrared spectra

Ganesh Chandan Kanakala, Bhuvanesh Sridharan and U. Deva Priyakumar*



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

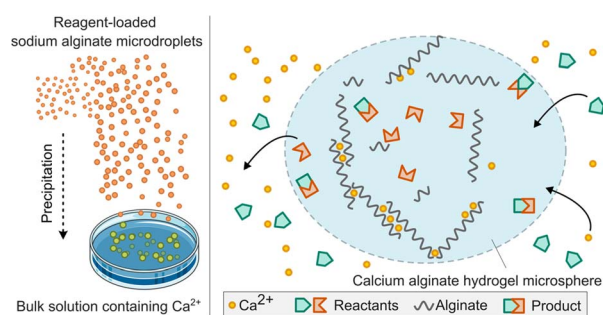


**SAVE
10%**

2424

In situ synthesis within micron-sized hydrogel reactors created via programmable aerosol chemistry

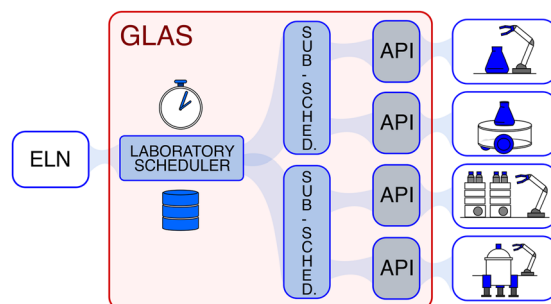
Luokun Zhang and S. Hessam M. Mehr*



2434

GLAS: an open-source easily expandable Git-based scheduling architecture for integral lab automation

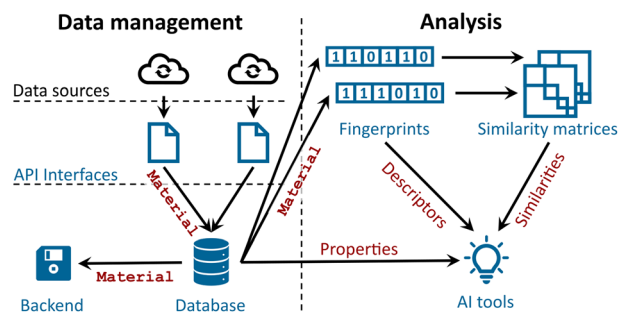
Jean-Charles Cousty, Tanguy Cavagna, Alec Schmidt, Edy Mariano, Keyan Villat, Florian de Nanteuil and Pascal Miéville*



2448

MADAS: a Python framework for assessing similarity in materials-science data

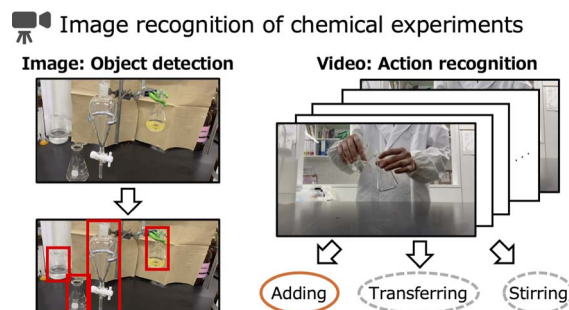
Martin Kuban,* Santiago Rigamonti and Claudia Draxl



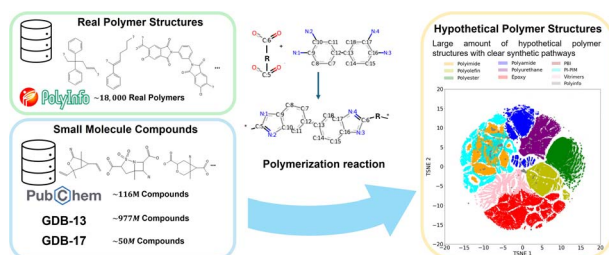
2458

Application of object detection and action recognition toward automated recognition of chemical experiments

Ryosuke Sasaki, Mikito Fujinami and Hiromi Nakai*



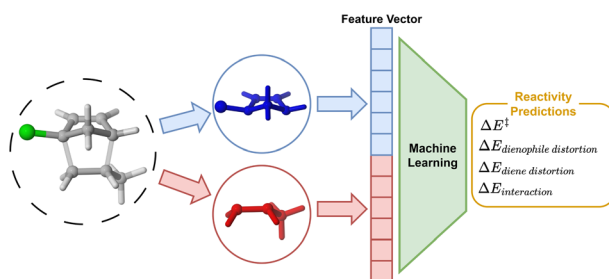
2465



Polyuniverse: generation of a large-scale polymer library using rule-based polymerization reactions for polymer informatics

Tianle Yue, Jianxin He and Ying Li*

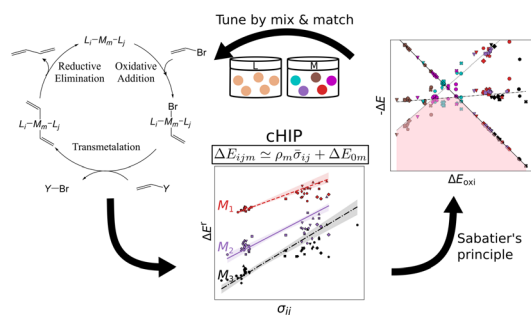
2479



Distortion/interaction analysis via machine learning

Samuel G. Espley, Samuel S. Allsop, David Buttar, Simone Tomasi and Matthew N. Grayson*

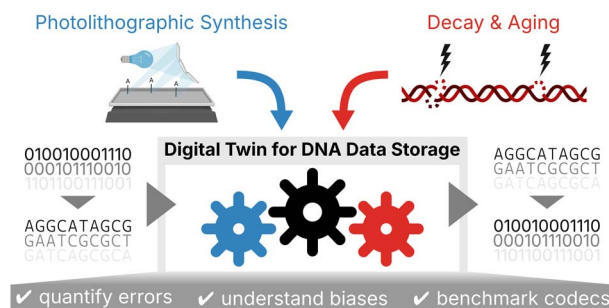
2487



Combining Hammett σ constants for Δ -machine learning and catalyst discovery

V. Diana Rakotonirina, Marco Bragato, Stefan Heinen and O. Anatole von Lilienfeld*

2497



Challenges for error-correction coding in DNA data storage: photolithographic synthesis and DNA decay

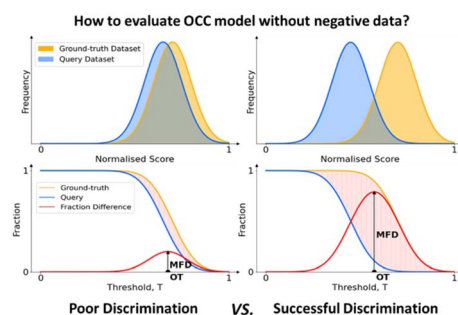
Andreas L. Gimpel, Wendelin J. Stark, Reinhard Heckel and Robert N. Grass*



2509

Accelerating metal–organic framework discovery via synthesisability prediction: the MFD evaluation method for one-class classification models

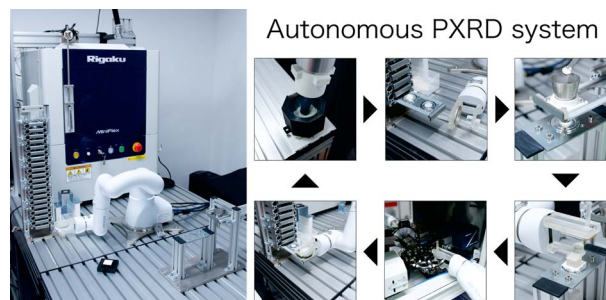
Chi Zhang, Dmytro Antypov, Matthew J. Rosseinsky and Matthew S. Dyer*



2523

Autonomous robotic experimentation system for powder X-ray diffraction

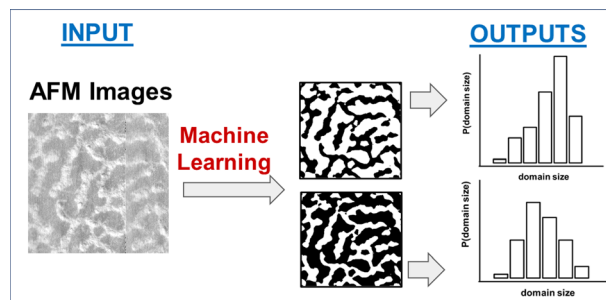
Yuto Yotsumoto, Yusaku Nakajima, Ryusei Takamoto, Yasuo Takeichi and Kanta Ono*



2533

Machine learning for analyzing atomic force microscopy (AFM) images generated from polymer blends

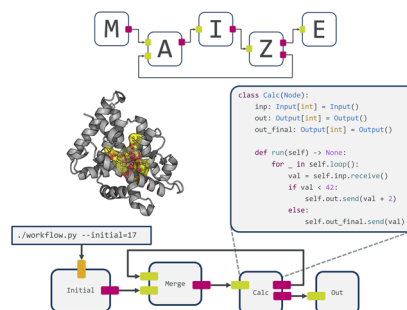
Aanish Paruchuri, Yunfei Wang, Xiaodan Gu and Arthi Jayaraman*



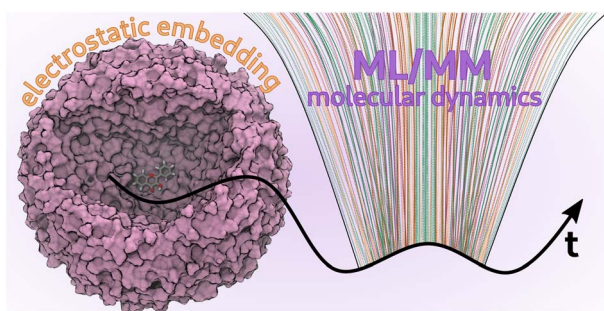
2551

Navigating the Maize: cyclic and conditional computational graphs for molecular simulation

Thomas Löhner,* Michele Assante, Michael Dodds, Lili Cao, Mikhail Kabeshov, Jon-Paul Janet, Marco Klähn and Ola Engkvist



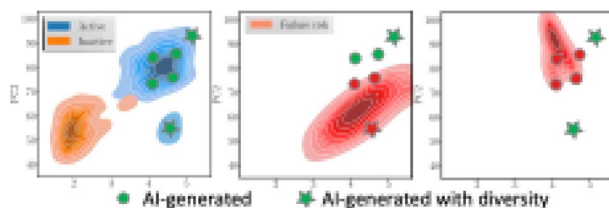
2560



Electrostatic embedding machine learning for ground and excited state molecular dynamics of solvated molecules

Patrizia Mazzeo,^{*} Edoardo Cignoni, Amanda Arcidiacono, Lorenzo Cupellini^{*} and Benedetta Mennucci

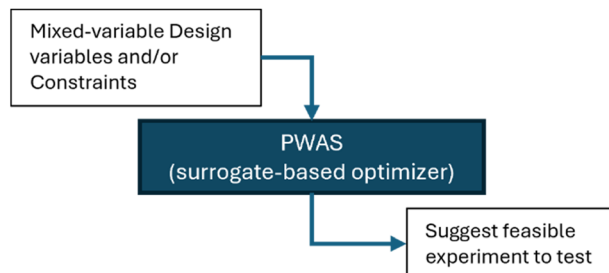
2572



Balancing exploration and exploitation in *de novo* drug design

Maxime Langevin, Marc Bianciotto^{*} and Rodolphe Vuilleumier^{*}

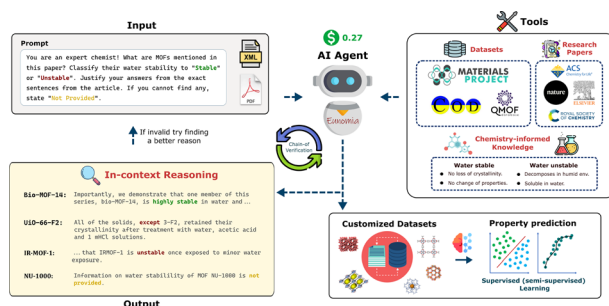
2589



Discrete and mixed-variable experimental design with surrogate-based approach

Mengjia Zhu, Austin Mroz, Lingfeng Gui, Kim E. Jelfs, Alberto Bemporad, Ehecatl Antonio del Río Chanona^{*} and Ye Seol Lee^{*}

2607



Agent-based learning of materials datasets from the scientific literature

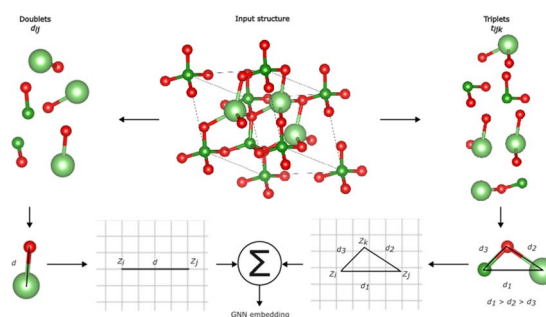
Mehrad Ansari and Seyed Mohamad Moosavi^{*}



2618

Embedding material graphs using the electron-ion potential: application to material fracture

Sherif Abdulkader Tawfik,* Tri Minh Nguyen, Salvy P. Russo, Truyen Tran, Sunil Gupta and Svetha Venkatesh



2628

Multi-objective synthesis optimization and kinetics of a sustainable terpolymer

Jin Da Tan, Andre K. Y. Low, Shannon Thoi Rui Ying, Sze Yu Tan, Wenguang Zhao, Yee-Fun Lim, Qianxiao Li, Saif A. Khan, Balamurugan Ramalingam* and Kedar Hippalgaonkar*

