

# Digital Discovery

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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

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### Unsupervised learning and pattern recognition in alloy design

Ninad Bhat, Nick Birbilis and Amanda S. Barnard\*

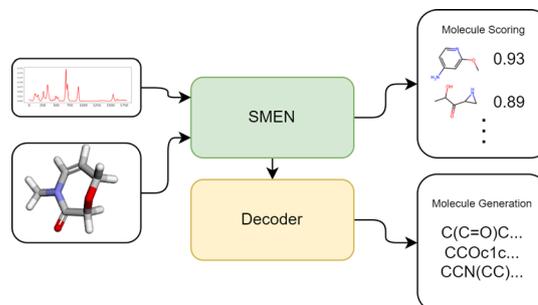


## COMMUNICATION

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### 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\*



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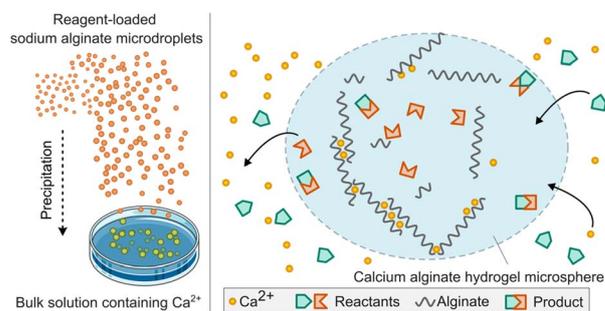


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## *In situ* synthesis within micron-sized hydrogel reactors created via programmable aerosol chemistry

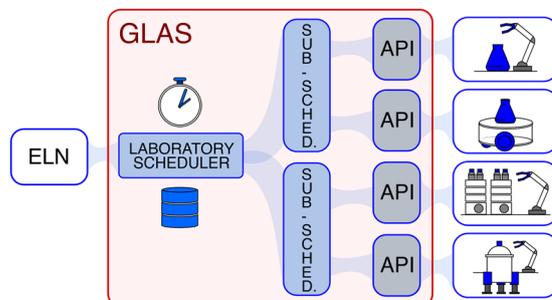
Luokun Zhang and S. Hessam M. Mehr\*



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

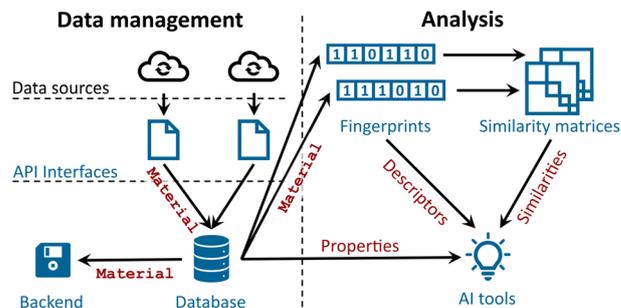
Jean-Charles Cousty, Tanguy Cavagna, Alec Schmidt, Edy Mariano, Keyan Villat, Florian de Nanteuil and Pascal Miéville\*



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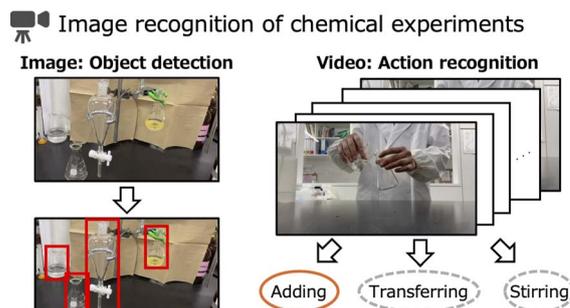
Martin Kuban,\* Santiago Rigamonti and Claudia Draxl



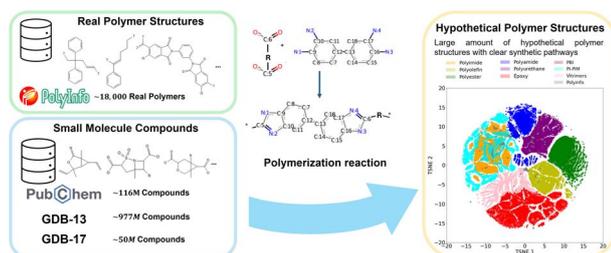
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## Application of object detection and action recognition toward automated recognition of chemical experiments

Ryosuke Sasaki, Mikito Fujinami and Hiromi Nakai\*



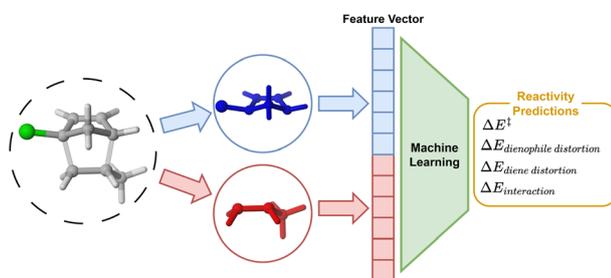
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## Polyuniverse: generation of a large-scale polymer library using rule-based polymerization reactions for polymer informatics

Tianle Yue, Jianxin He and Ying Li\*

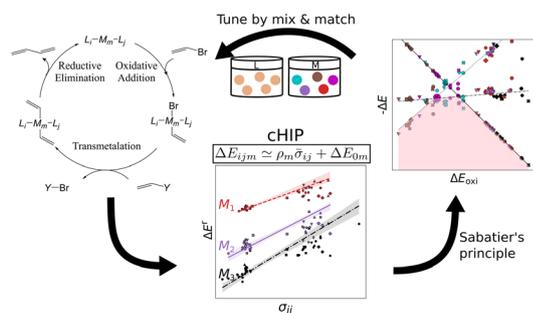
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## Distortion/interaction analysis via machine learning

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

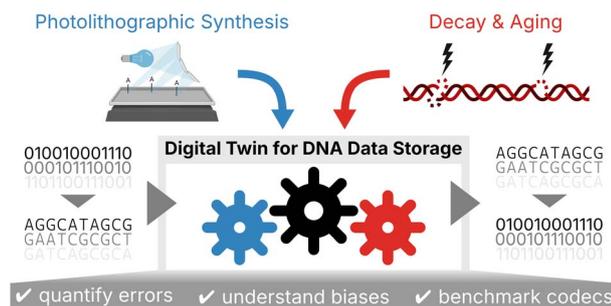
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## Combining Hammett $\sigma$ constants for $\Delta$ -machine learning and catalyst discovery

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

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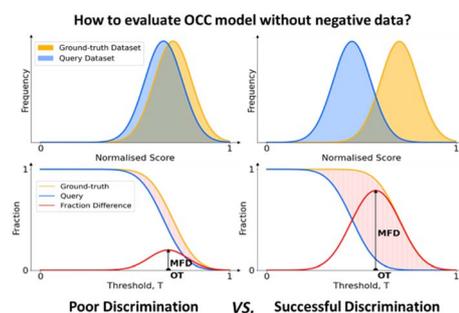
Andreas L. Gimpel, Wendelin J. Stark, Reinhard Heckel and Robert N. Grass\*



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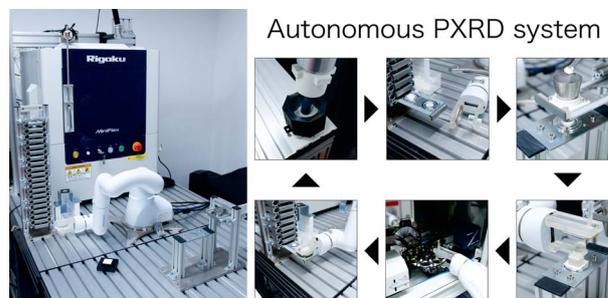
Chi Zhang, Dmytro Antypov, Matthew J. Rosseinsky and Matthew S. Dyer\*



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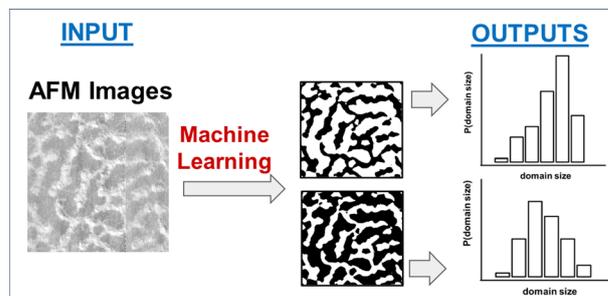
Yuto Yotsumoto, Yusaku Nakajima, Ryusei Takamoto, Yasuo Takeichi and Kanta Ono\*



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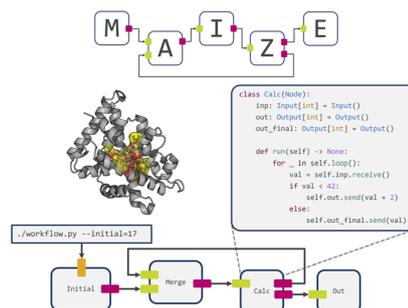
Aanish Paruchuri, Yunfei Wang, Xiaodan Gu and Arthi Jayaraman\*



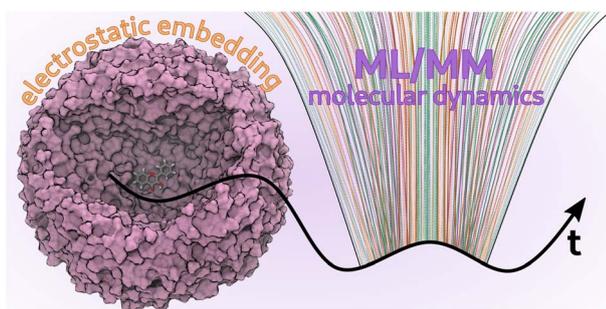
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## Navigating the Maize: cyclic and conditional computational graphs for molecular simulation

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



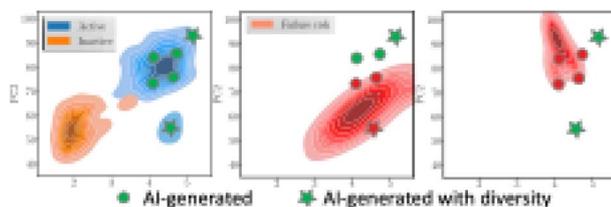
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### Electrostatic embedding machine learning for ground and excited state molecular dynamics of solvated molecules

Patrizia Mazzeo,<sup>\*</sup> Edoardo Cignoni, Amanda Arcidiacono, Lorenzo Cupellini<sup>\*</sup> and Benedetta Mennucci

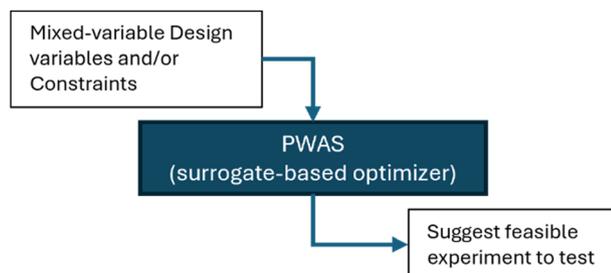
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### Balancing exploration and exploitation in *de novo* drug design

Maxime Langevin, Marc Bianciotto<sup>\*</sup> and Rodolphe Vuilleumier<sup>\*</sup>

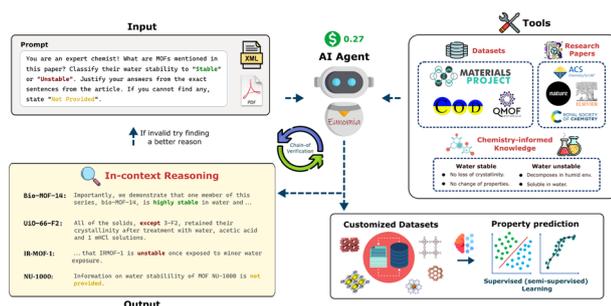
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### Discrete and mixed-variable experimental design with surrogate-based approach

Mengjia Zhu, Austin Mroz, Lingfeng Gui, Kim E. Jelfs, Alberto Bemporad, Ehecatl Antonio del Río Chanona<sup>\*</sup> and Ye Seol Lee<sup>\*</sup>

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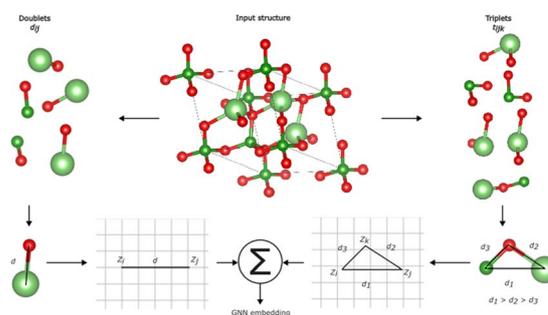
Mehrad Ansari and Seyed Mohamad Moosavi<sup>\*</sup>



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## 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



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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\*

