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ISSN 2635-098X CODEN DDIIAI 3(12) 2387–2638 (2024)



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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.



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Unsupervised learning and pattern recognition in alloy design

Ninad Bhat, Nick Birbilis and Amanda S. Barnard*

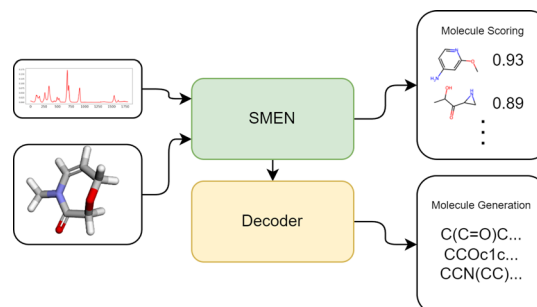


COMMUNICATION

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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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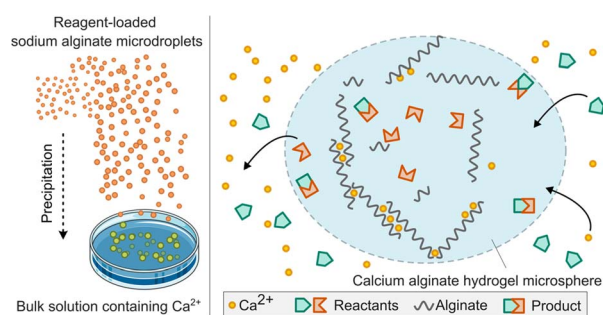


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In situ synthesis within micron-sized hydrogel reactors created via programmable aerosol chemistry

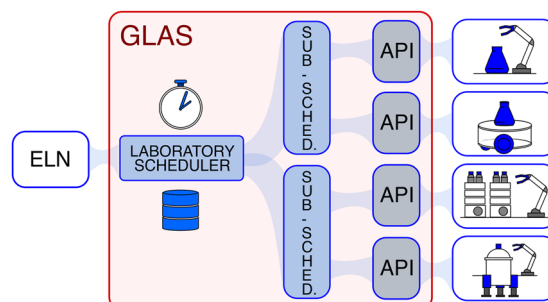
Luokun Zhang and S. Hessam M. Mehr*



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

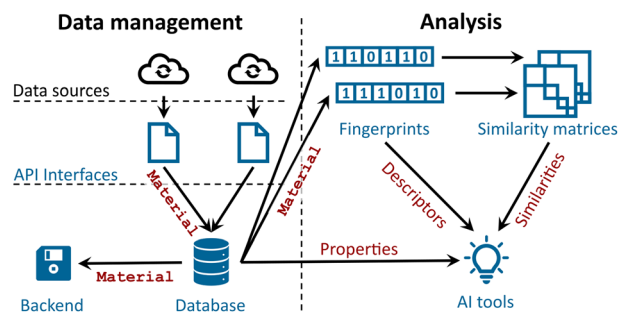
Jean-Charles Cousty, Tanguy Cavagna, Alec Schmidt, Edy Mariano, Keyan Villat, Florian de Nanteuil and Pascal Miéville*



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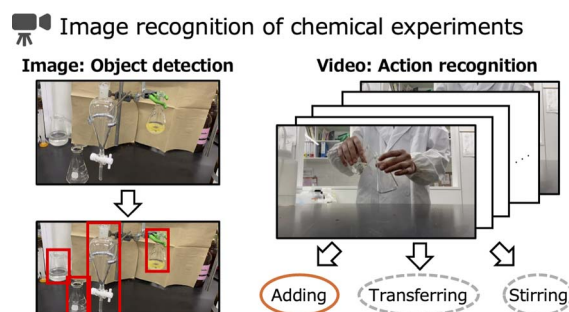
Martin Kuban,* Santiago Rigamonti and Claudia Draxl



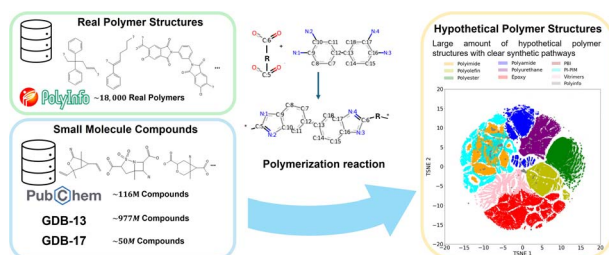
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Application of object detection and action recognition toward automated recognition of chemical experiments

Ryosuke Sasaki, Mikito Fujinami and Hiromi Nakai*



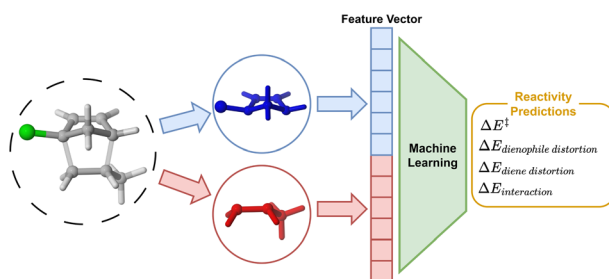
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Polyuniverse: generation of a large-scale polymer library using rule-based polymerization reactions for polymer informatics

Tianle Yue, Jianxin He and Ying Li*

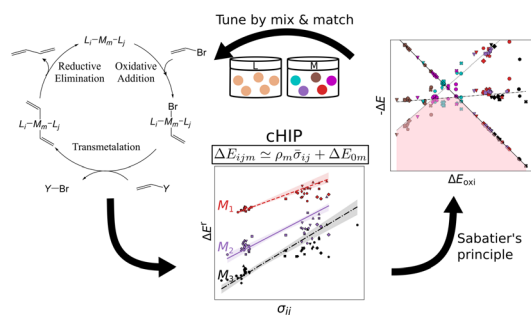
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Distortion/interaction analysis via machine learning

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

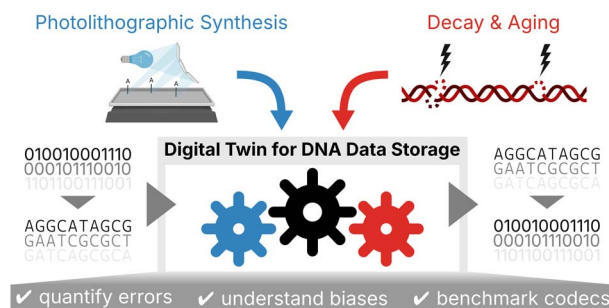
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V. Diana Rakotonirina, Marco Bragato, Stefan Heinen and O. Anatole von Lilienfeld*

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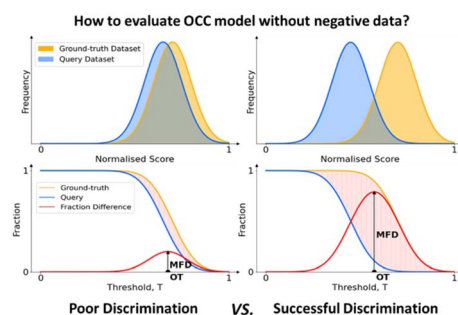
Andreas L. Gimpel, Wendelin J. Stark, Reinhard Heckel and Robert N. Grass*



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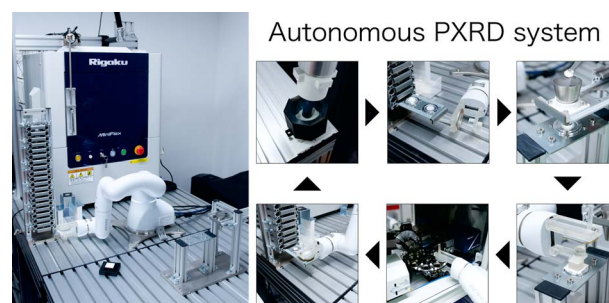
Chi Zhang, Dmytro Antypov, Matthew J. Rosseinsky and Matthew S. Dyer*



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Autonomous robotic experimentation system for powder X-ray diffraction

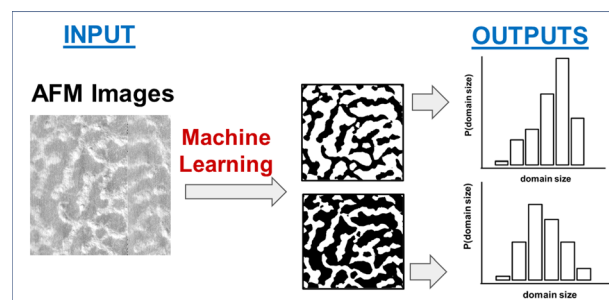
Yuto Yotsumoto, Yusaku Nakajima, Ryusei Takamoto, Yasuo Takeichi and Kanta Ono*



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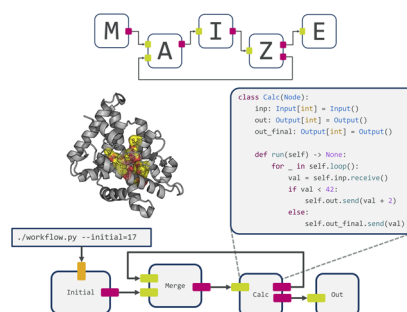
Aanish Paruchuri, Yunfei Wang, Xiaodan Gu and Arthi Jayaraman*



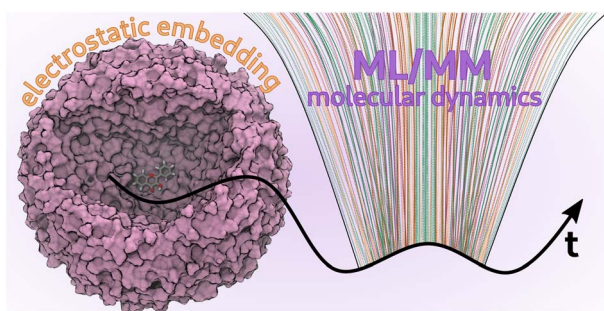
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Navigating the Maize: cyclic and conditional computational graphs for molecular simulation

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



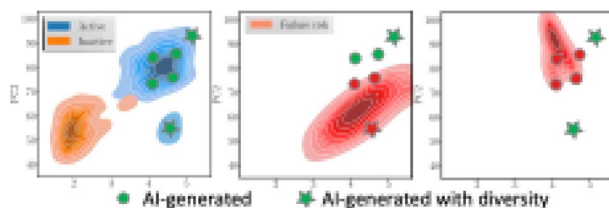
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Electrostatic embedding machine learning for ground and excited state molecular dynamics of solvated molecules

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

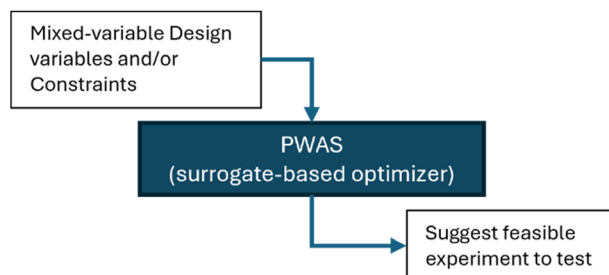
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Balancing exploration and exploitation in *de novo* drug design

Maxime Langevin, Marc Bianciotto* and Rodolphe Vuilleumier*

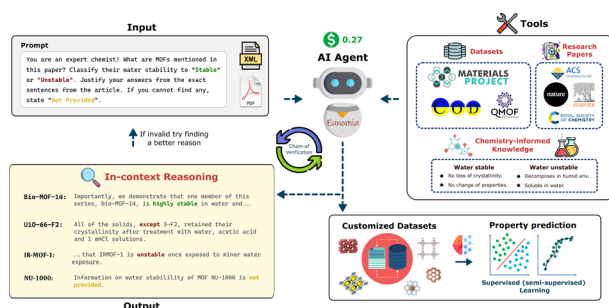
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Discrete and mixed-variable experimental design with surrogate-based approach

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Agent-based learning of materials datasets from the scientific literature

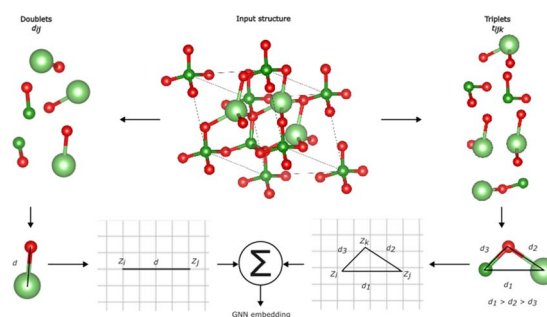
Mehrad Ansari and Seyed Mohamad Moosavi*



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



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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*

