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Ninad Bhat, Nick Birbilis and Amanda S. Barnard*

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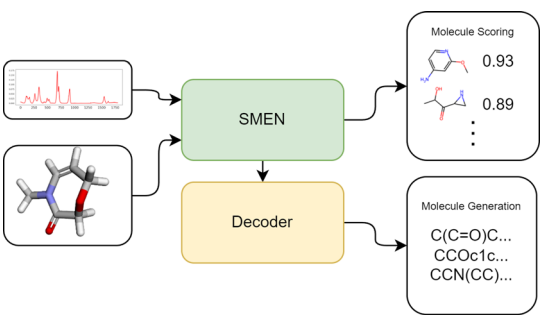
Ganesh Chandan Kanakala, Bhuvanesh Sridharan and U. Deva Priyakumar*



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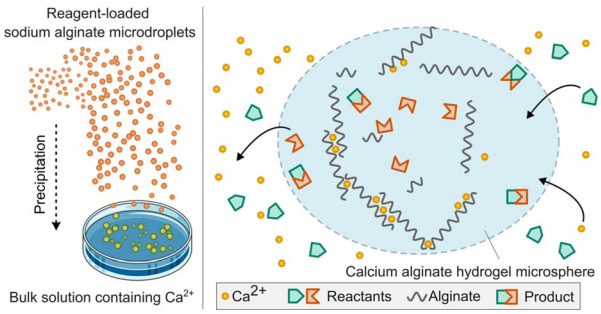
PAPERS

2424

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

Luokun Zhang and S. Hessam M. Mehr*



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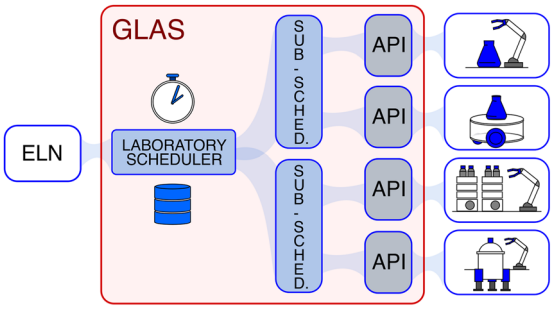
GLAS: an open-source easily expandable Git-based scheduling architecture for integral lab automation

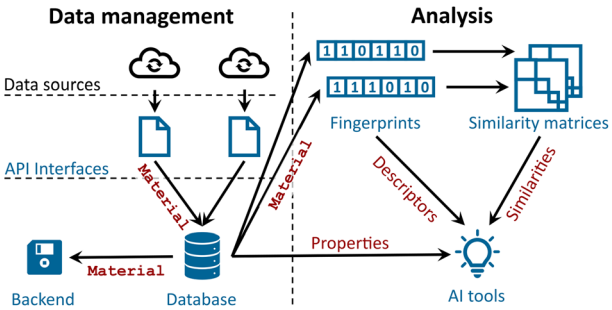
Jean-Charles Cousty, Tanguy Cavagna, Alec Schmidt, Edy Mariano, Keyan Villat, Florian de Nanteuil and Pascal Miéville*



2448

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

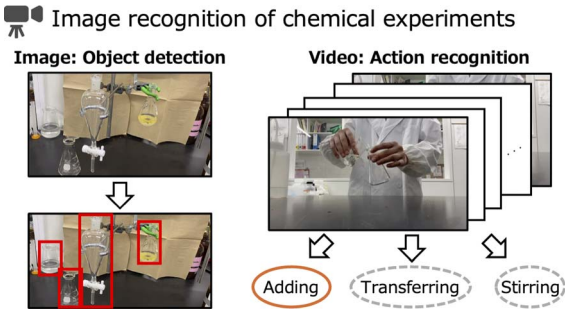
Martin Kuban,* Santiago Rigamonti and Claudia Draxl



2458

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

Ryosuke Sasaki, Mikito Fujinami and Hiromi Nakai*



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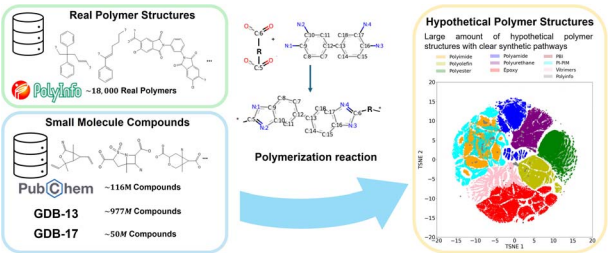

Polyuniverse: generation of a large-scale polymer library using rule-based polymerization reactions for polymer informatics

Tianle Yue, Jianxin He and Ying Li*

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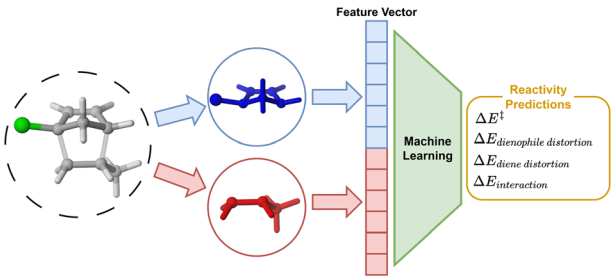

Distortion/interaction analysis *via* machine learning

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

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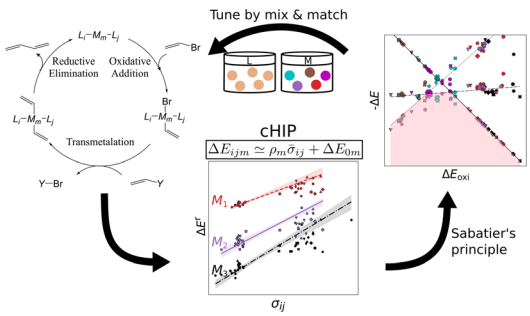

Combining Hammett σ constants for Δ-machine learning and catalyst discovery

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

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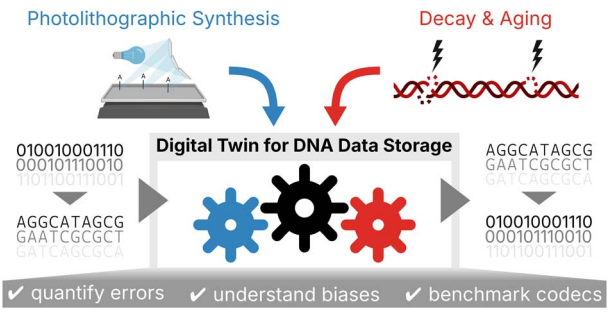

Challenges for error-correction coding in DNA data storage: photolithographic synthesis and DNA decay

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

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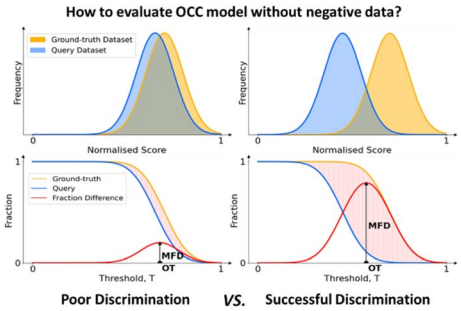
Accelerating metal–organic framework discovery *via* synthesisability prediction: the MFD evaluation method for one-class classification models

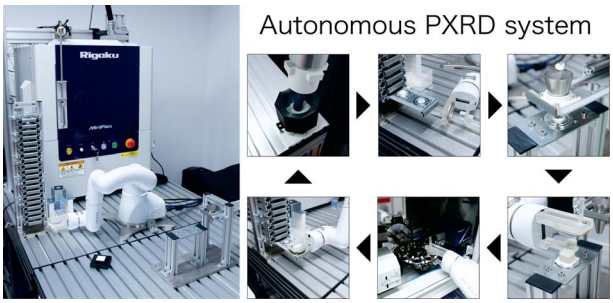
Chi Zhang, Dmytro Antypov, Matthew J. Rosseinsky and Matthew S. Dyer*



2523

Autonomous robotic experimentation system for powder X-ray diffraction

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



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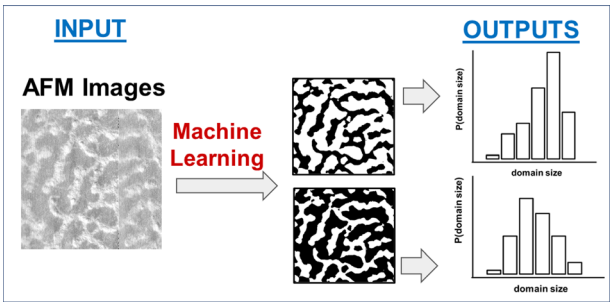
Machine learning for analyzing atomic force microscopy (AFM) images generated from polymer blends

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



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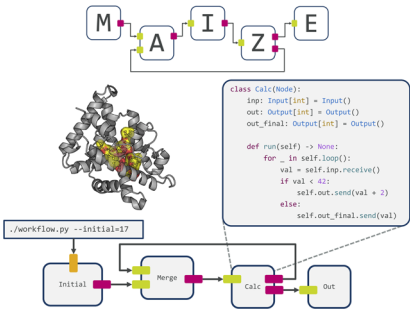
Navigating the Maize: cyclic and conditional computational graphs for molecular simulation

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



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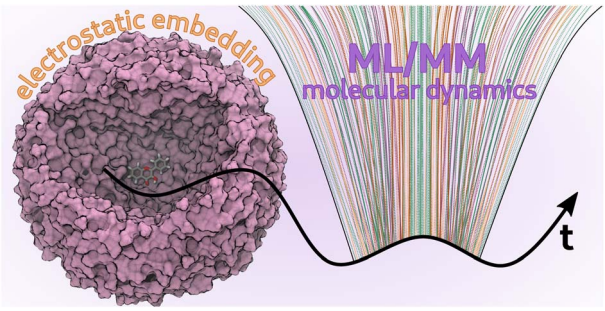

Electrostatic embedding machine learning for ground and excited state molecular dynamics of solvated molecules

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

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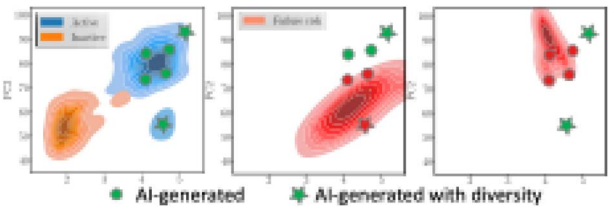

Balancing exploration and exploitation in *de novo* drug design

Maxime Langevin, Marc Bianciotto* and Rodolphe Vuilleumier*

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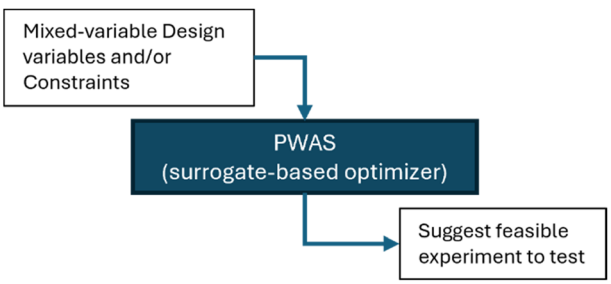

Discrete and mixed-variable experimental design with surrogate-based approach

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

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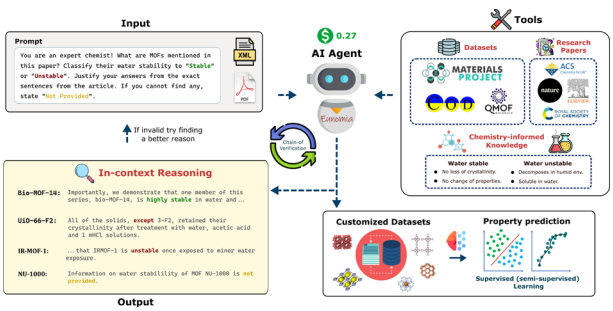

Agent-based learning of materials datasets from the scientific literature

Mehrad Ansari and Seyed Mohamad Moosavi*

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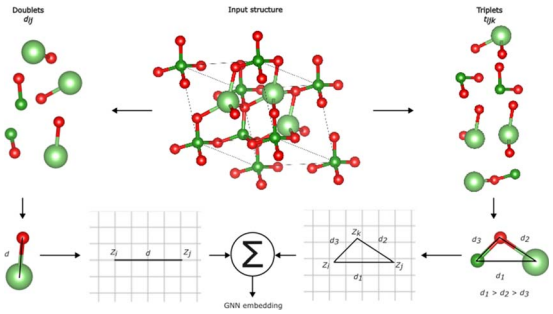
Embedding material graphs using the electron-ion potential: application to material fracture

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



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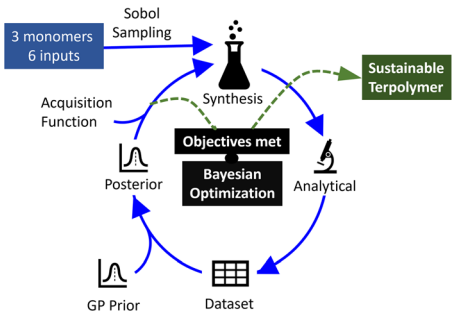
Multi-objective synthesis optimization and kinetics of a sustainable terpolymer

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*