

# Digital Discovery

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## IN THIS ISSUE

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**Cover**  
See Niaz Abdolrahim *et al.*, pp. 1991–2015. Image reproduced by permission of Niaz Abdolrahim and Ali Vosoughi from *Digital Discovery*, 2026, 5, 1991. Image generated using Google Gemini.



**Inside cover**  
See Jaeyune Ryu, Yousung Jung *et al.*, pp. 1968–1980. Image reproduced by permission of Yousung Jung from *Digital Discovery*, 2026, 5, 1968. Image generated using Google Gemini.

## EDITORIAL

1962

First annual *Digital Discovery* Emerging Investigators collection



## PROFILE

1963

Contributors to the *Digital Discovery* Emerging Investigators collection 2025



# RSC Applied Polymers

GOLD  
OPEN  
ACCESS

The application of polymers,  
both natural and synthetic

Interdisciplinary and open access

[rsc.li/RSCApplPolym](https://rsc.li/RSCApplPolym)

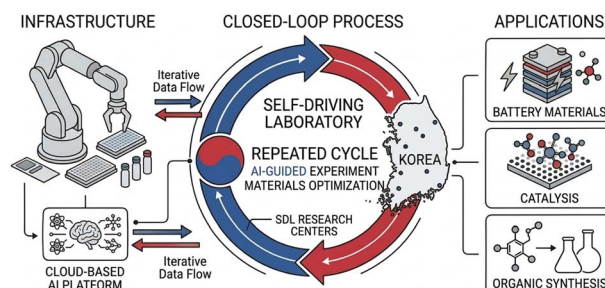
Fundamental questions  
Elemental answers

## PERSPECTIVE

1968

**Self-driving laboratories in Korea: a new era of autonomous discovery**

Jiho Hwang, Seongmin Kim, Sooyoun Lim, Juhwan Kim, Seungwoo Lee, Seonghyeon Min, Jisoo Song, Jeongwook Lim, Seonghun Hong, Jin-Ha Hwang, Youn-Suk Choi, Dong-Hwa Seo, Sang Soo Han, KangGeon Kim, Su-Hyun Yoo, Jungho Shin, Jang Wook Choi, Jaewook Nam, Jungwon Park, Jaeyune Ryu\* and Yousung Jung\*

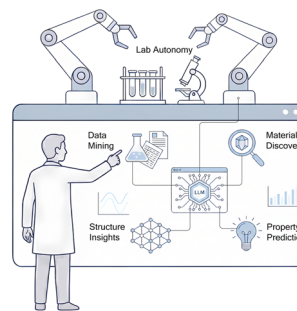


## REVIEW

1981

**Large language models in materials science and the need for open-source approaches**

Fengxu Yang, Weitong Chen and Jack D. Evans\*

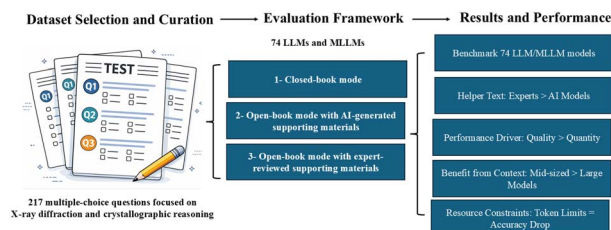


## PAPERS

1991

**OPENXRD: a comprehensive benchmark framework for LLM/MLLM XRD question answering**

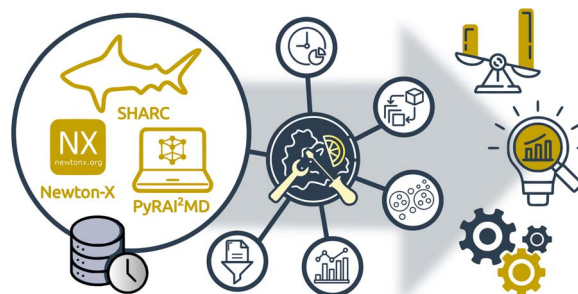
Ali Vosoughi, Ayoub Shahnazari, Yufeng Xi, Zeliang Zhang, Griffin Hess, Chenliang Xu and Niaz Abdolrahim\*



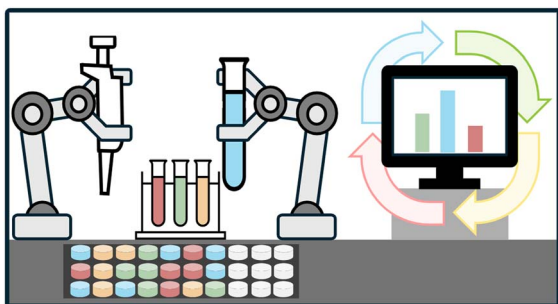
2016

**shnitsel-tools: a toolkit for the full lifecycle of surface hopping trajectory data**

Kevin Höllring, Theodor E. Röhrkasten and Carolin Müller\*



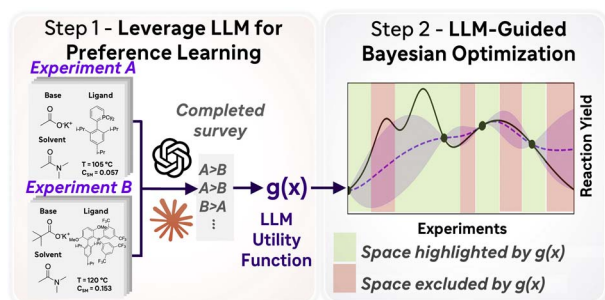
2028



### A user's guide to your first self-driving liquid handling lab

Apostolos P. Maroulis, Dylan M. Waynor, Quinn M. Gallagher, Roshan A. Patel, Matthew Tamasi, D. Christopher Radford, Michael A. Webb\* and Adam J. Gormley\*

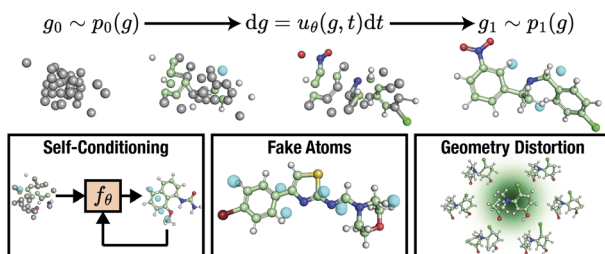
2042



### Distilling and exploiting quantitative insights from large language models for enhanced Bayesian optimization of chemical reactions

Roshan A. Patel, Mingxuan Li, Chin-Fei Chang, Louis De Lescure, Paul Chauvin, Alan Cherney, Saeed Moayedpour, Sven Jager and Yasser Jangjou\*

2052

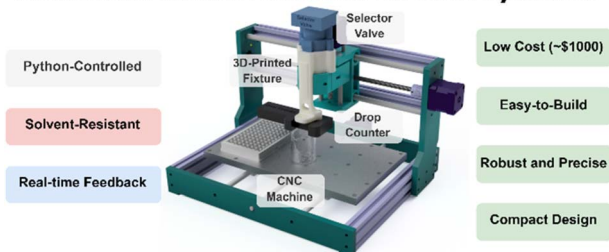


### FlowMol3: flow matching for 3D *de novo* small-molecule generation

Ian Dunn and David R. Koes\*

2067

### Automated Fraction Collector for Flow Synthesis



### Python-controlled, solvent-resistant fraction collector for automated flow synthesis

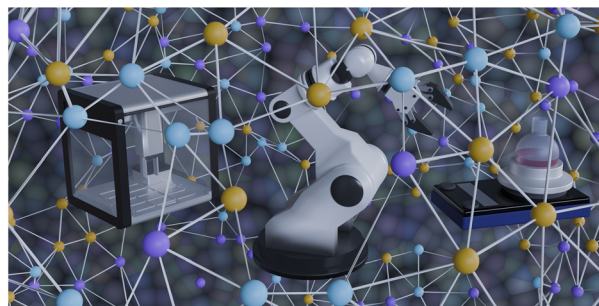
Hongchen Wang, Owen A. Meville, Harrison A. Mills, Monique Ngan, Jay R. Werber and Nipun Kumar Gupta\*



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### WeChemSynOntology: semantic modeling of wet chemical syntheses in a self-driving lab for nano- and advanced materials

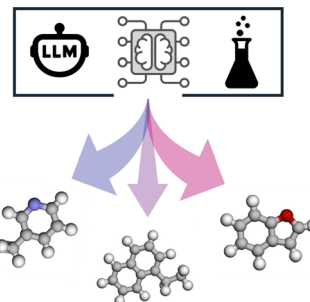
Markus Schilling, Harald Bresch, Bernd Bayerlein\* and Bastian Ruehle\*



2089

### Discovery of hydrogen storage molecules using large language models and machine learning

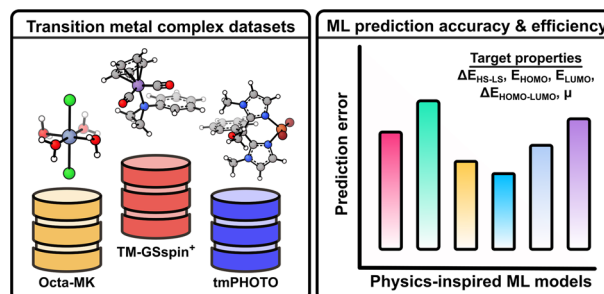
Hassan Harb,\* Magali S. Ferrandon, Timothy A. Goetjen, Seryeong Lee, Omar K. Farha, Massimiliano Delferro and Rajeev Surendran Assary\*



2103

### Benchmarking physics-inspired machine learning models for transition metal complexes with diverse charge and spin states

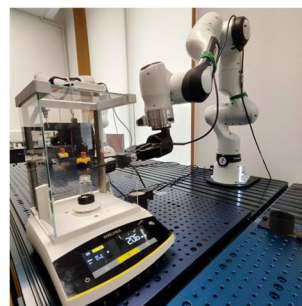
Yuri Cho, Ksenia R. Briling, Yannick Calvino Alonso, Ruben Laplaza and Clemence Corminboeuf\*



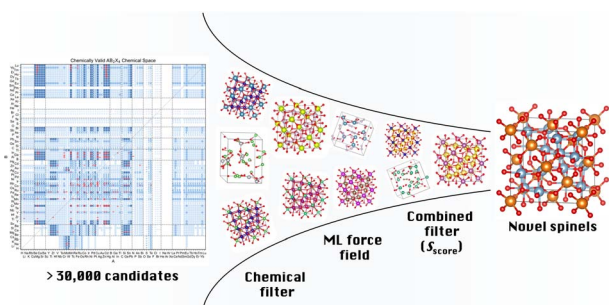
2120

### Vision-guided adaptive scooping for powder weighing in autonomous chemistry laboratories

Nikola Radulov, Thomas Little, Andrew I. Cooper and Gabriella Pizzuto\*



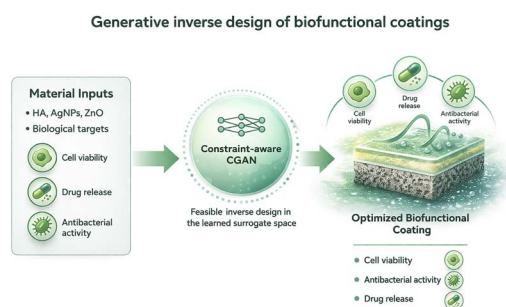
2128



### Data-driven exploration of $AB_2X_4$ ( $X = O, S, Se, Te$ ) spinel chemical space

Panyalak Detrattanawichai, Zhenzhu Li, Hyunsoo Park, Kinga O. Mastej and Aron Walsh\*

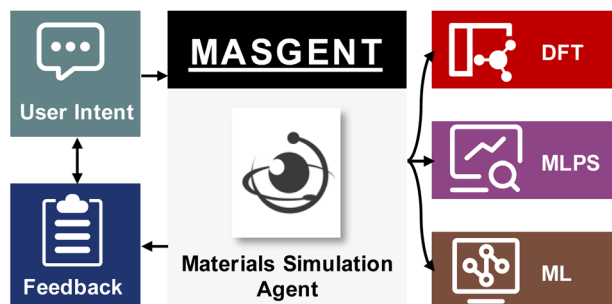
2137



### Deep generative inverse design of biofunctional polymer coatings using conditional GANs

Wafa Benaatou,\* Mudasir Ahmad Wani and Kashish Ara Shakil

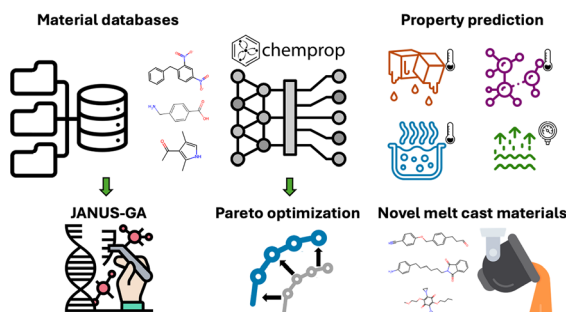
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### Masgent: an AI-assisted materials simulation agent

Guangchen Liu, Songge Yang and Yu Zhong\*

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### A deep learning approach to searching property spaces of materials

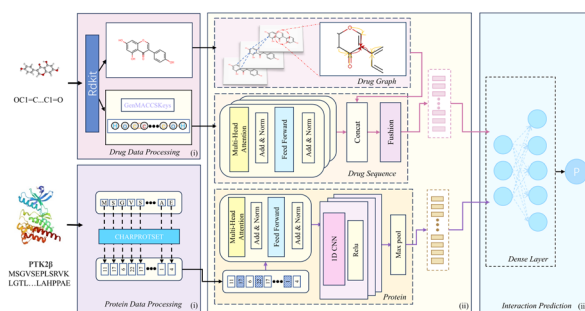
Robert J. Appleton, Brian C. Barnes, Steven F. Son and Alejandro Strachan\*



2184

## MolRes-DTA: a molecular-multiview fusion and residue-aware model for drug-target affinity prediction

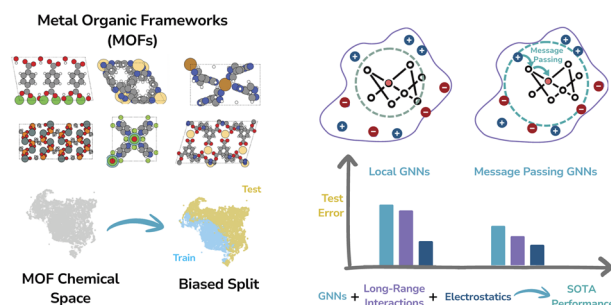
Hongli Hou, Qi Wei, Dian Huang,\* Minglu Zhao, Hongliang Duan and Shengzhong Feng\*



2195

## Generalization of long-range machine learning potentials in complex chemical spaces

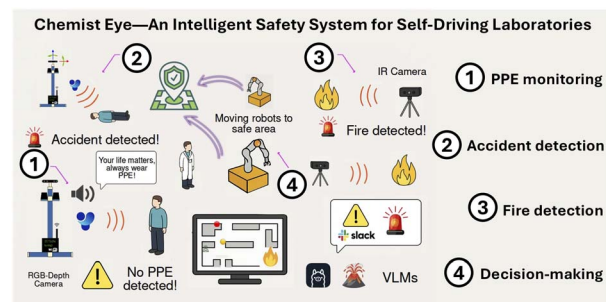
Michał Sanocki and Julija Zavadlav\*



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## Chemist Eye: a visual language model-powered system for safety monitoring and robot decision-making in self-driving laboratories

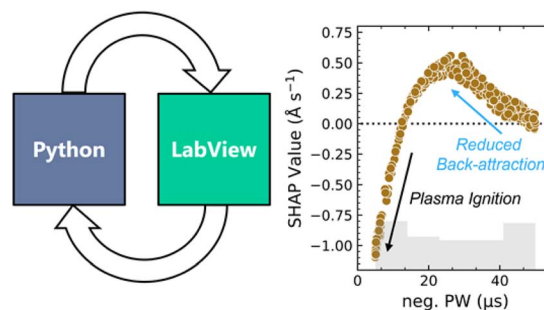
Francisco Munguia-Galeano, Zhengxue Zhou, Satheeshkumar Veeramani, Hatem Fakhrudeen, Louis Longley, Rob Clowes and Andrew I. Cooper\*



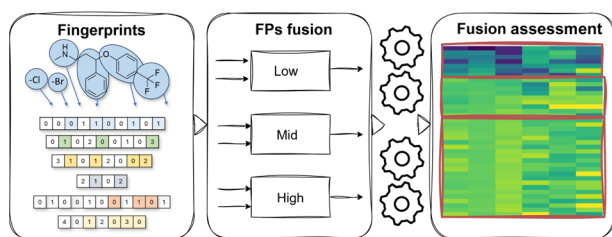
2221

## Autonomous sampling and SHAP interpretation of deposition-rates in bipolar HiPIMS

Alexander Wieczorek, Nathan Rodkey,\* Jan Sommerhäuser, Jason Hatrick-Simpers and Sebastian Siot\*



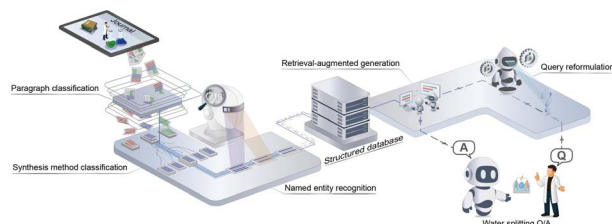
2232



### Enhancing predictive modeling with molecular fingerprint fusion strategies

Viktoria Turkina,<sup>\*</sup> Melanie R. W. Messih, Etienne Kant, Jelle T. Gringhuis, Annemieke Petrignani, Garry Corthals, Jake W. O'Brien and Saer Samanipour<sup>\*</sup>

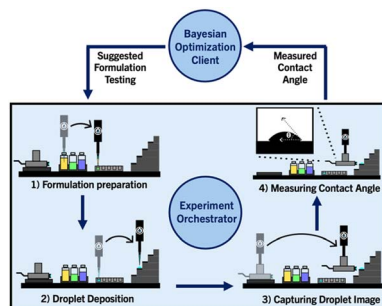
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### Structured domain knowledge enables trustworthy materials science question-answering with large language models

Daegun Lee, Jiwoo Choi, Gyeong Hoon Yi, Seok Su Sohn, Byungju Lee<sup>\*</sup> and Donghun Kim<sup>\*</sup>

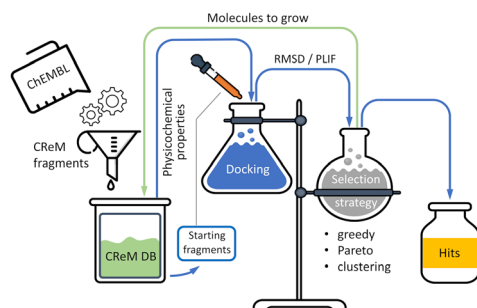
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### RAISE: a self-driving laboratory for interfacial property formulation discovery

Mohammad Nazari, Sheldon Mei, Jeffrey Watchorn, Alex Zhang, Erin Ng, Tao Wen, Abhijoy Mandal, Kevin Golovin, Alán Aspuru-Guzik and Frank Gu<sup>\*</sup>

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### CReM-dock: *de novo* design of synthetically feasible structures guided by molecular docking

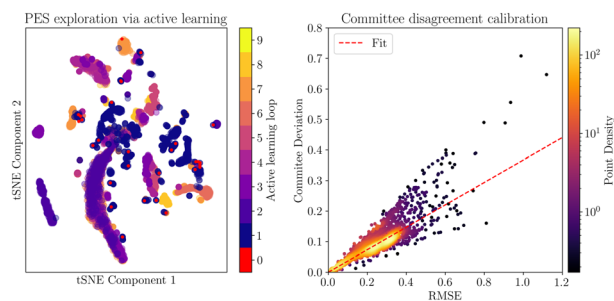
Guzel Minibaeva, Haolin Du, Finlay Clark, Julien Michel and Pavel Polishchuk<sup>\*</sup>



2292

## AiiDA-TrainsPot: towards automated training of neural-network interatomic potentials

Davide Bidoggia,<sup>\*</sup> Nataliia Manko, Maria Peressi and Antimo Marrazzo<sup>\*</sup>



2310

## Accelerating discovery across scientific disciplines through reproducible workflows with AiiDALab

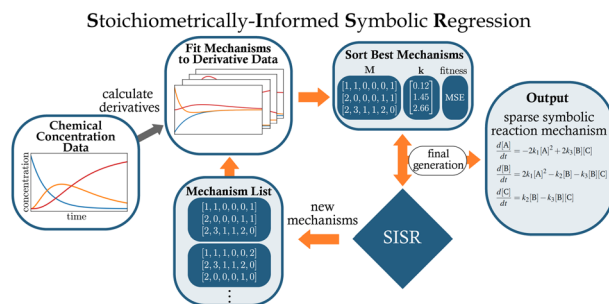
Aliaksandr V. Yakutovich, Daniel Hollas, Edan Bainglass, Jusong Yu, Corsin Battaglia, Miki Bonacci, Lucas Fernandez Vilanova, Stephan Henne, Anders Kaestner, Michel Kenzelmann, Graham Kimbell, Jakob Lass, Fabio Lopes, Daniel G. Mazzone, Andres Ortega-Guerrero, Xing Wang,<sup>\*</sup> Nicola Marzari, Carlo A. Pignedoli<sup>\*</sup> and Giovanni Pizzi<sup>\*</sup>



2325

## Stoichiometrically-informed symbolic regression for extracting chemical reaction mechanisms from data

Manuel Palma Banos, Joel D. Kress, Rigoberto Hernandez and Galen T. Craven<sup>\*</sup>



2342

## Uncertainty-aware active learning reveals reliability limits in lead-free halide perovskite screening

Xiyao Yu<sup>\*</sup>

