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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

PROFILE

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Fundamental questions
Elemental answers

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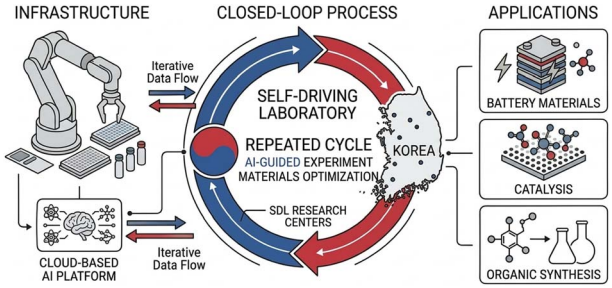
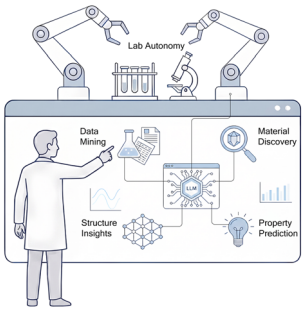
PERSPECTIVE



REVIEW



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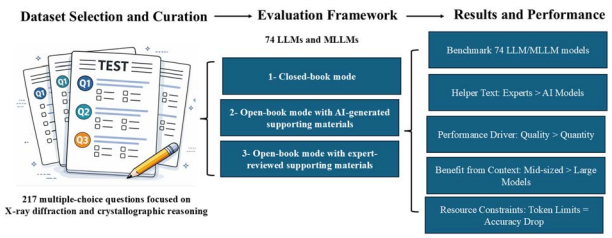

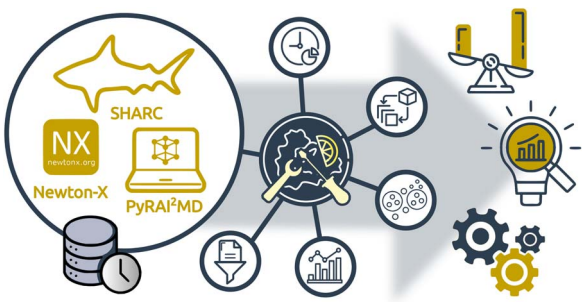

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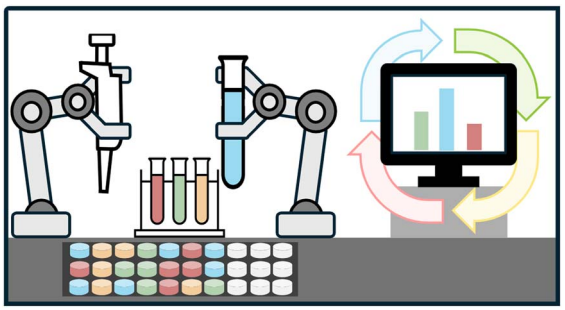
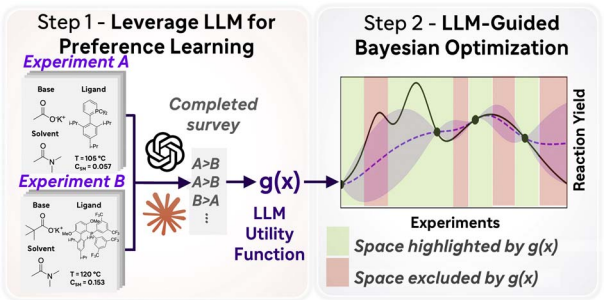
2028



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*

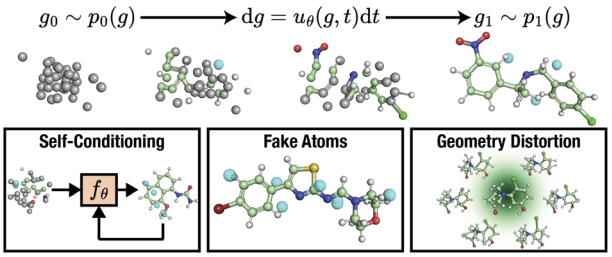
2042



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*

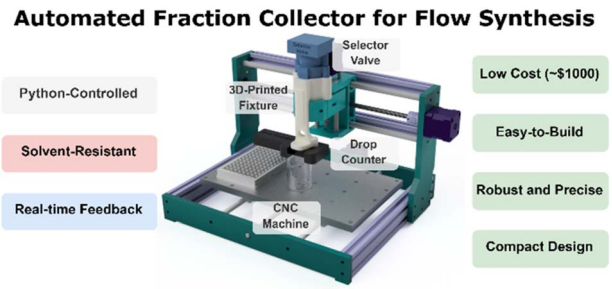
2052



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

Ian Dunn and David R. Koes*

2067



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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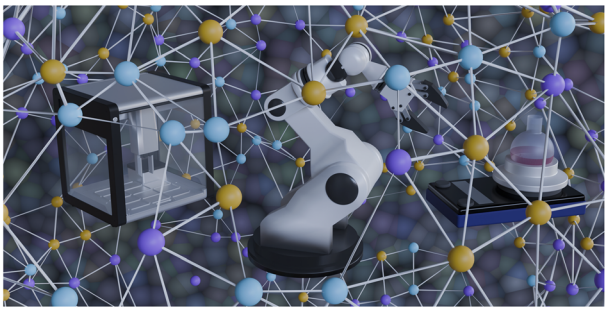

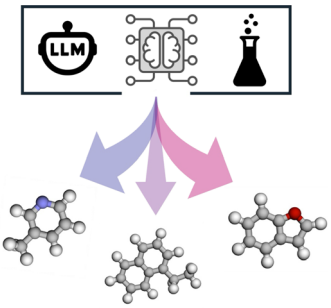

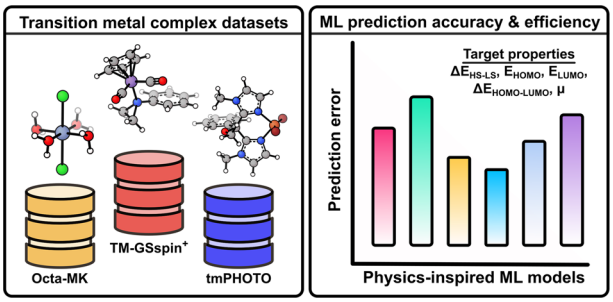

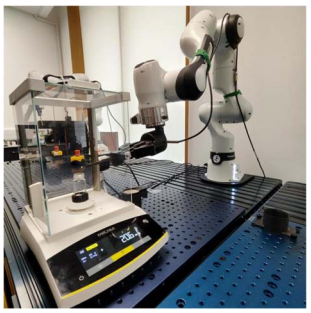

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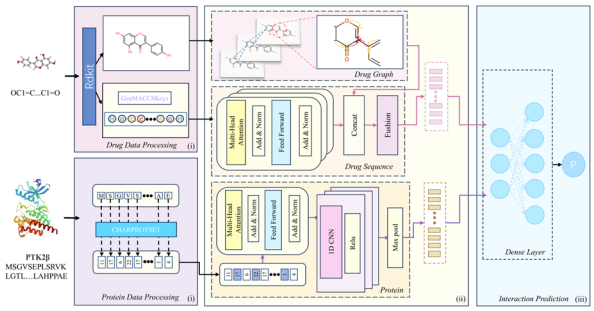
MolRes-DTA: a molecular-multiview fusion and residue-aware model for drug-target affinity prediction

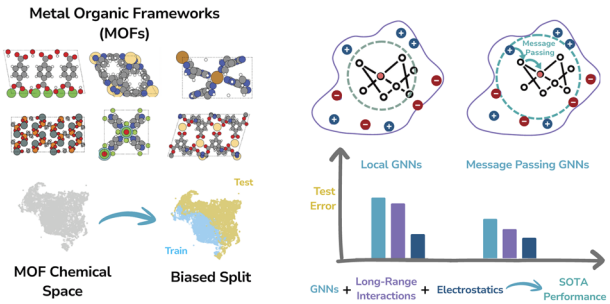
Hongli Hou, Qi Wei, Dian Huang,* Minglu Zhao, Hongliang Duan and Shengzhong Feng*



2195

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

Michał Sanocki and Julija Zavadlav*



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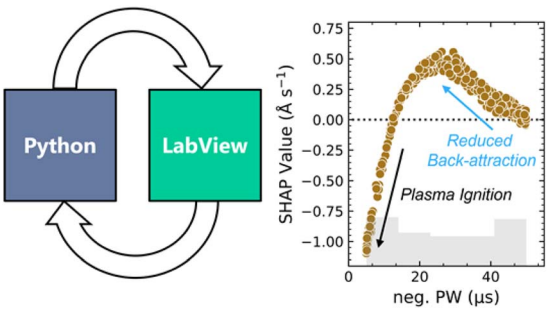
Chemist Eye: a visual language model-powered system for safety monitoring and robot decision-making in self-driving laboratories

Francisco Munguia-Galeano, Zhengxue Zhou, Satheeshkumar Veeramani, Hatem Fakhruldeen, 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 Hattrick-Simpers and Sebastian Siol*



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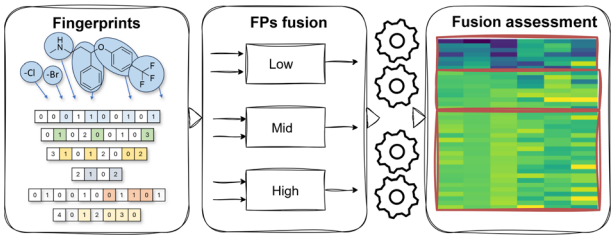
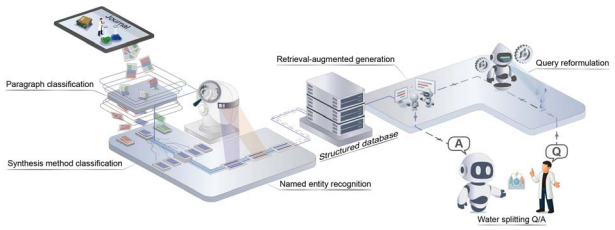


Enhancing predictive modeling with molecular fingerprint fusion strategies

Viktoriia Turkina,* Melanie R. W. Messih, Etienne Kant, Jelle T. Gringhuis, Annemieke Petrignani, Garry Corthals, Jake W. O'Brien and Saer Samanipour*

2243



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* and Donghun Kim*

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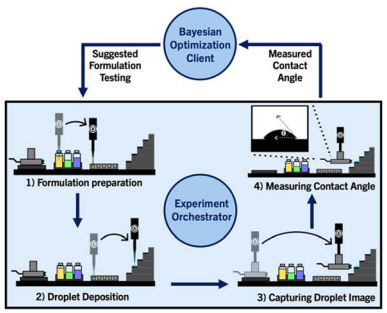

RAISE: a self-driving laboratory for interfacial property formulation discovery

Mohammad Nazeri, Sheldon Mei, Jeffrey Watchorn, Alex Zhang, Erin Ng, Tao Wen, Abhijoy Mandal, Kevin Golovin, Alán Aspuru-Guzik and Frank Gu*

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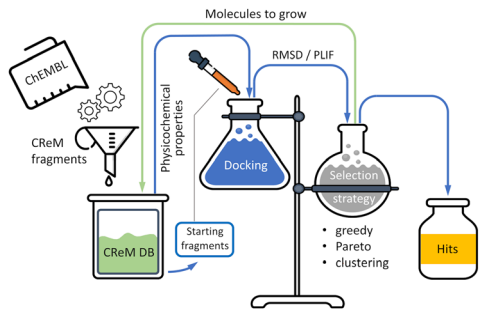

CReM-dock: *de novo* design of synthetically feasible structures guided by molecular docking

Guzel Minibaeva, Haolin Du, Finlay Clark, Julien Michel and Pavel Polishchuk*

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