

IN THIS ISSUE

ISSN 2635-098X CODEN DDIIAI 4(4) 883–1114 (2025)



Cover

See Alexander E. Siemenn, Tonio Buonassisi *et al.*, pp. 896–909. Image reproduced by permission of Alexander E. Siemenn and Matthew Siemenn from *Digital Discovery*, 2025, 4, 896.



Inside cover

See Ying Li *et al.*, pp. 910–926. Image reproduced by permission of Zoe Zhou and Tianle Yue from *Digital Discovery*, 2025, 4, 910.

OPINION

892

Digital discovery and the new experimental frontier

S. Hessam M. Mehr

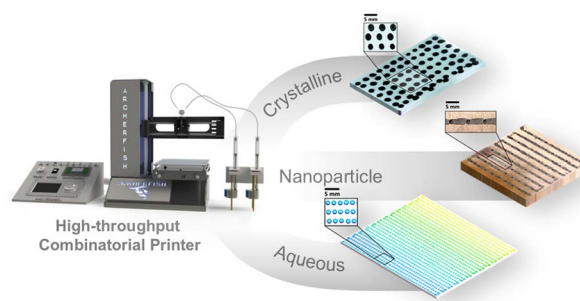


PAPERS

896

Archerfish: a retrofitted 3D printer for high-throughput combinatorial experimentation via continuous printing

Alexander E. Siemenn,* Basita Das, Eunice Aissi, Fang Sheng, Lleyton Elliott, Blake Hudspeth, Marilyn Meyers, James Serdy and Tonio Buonassisi*



Advance your career in science

with professional recognition that showcases
your **experience, expertise and dedication**

Stand out from the crowd

Prove your commitment
to attaining excellence in
your field

Gain the recognition you deserve

Achieve a professional
qualification that inspires
confidence and trust

Unlock your career potential

Apply for our professional
registers (RSci, RSciTech)
or chartered status
(CChem, CSci, CEnv)

Apply now

rsc.li/professional-development

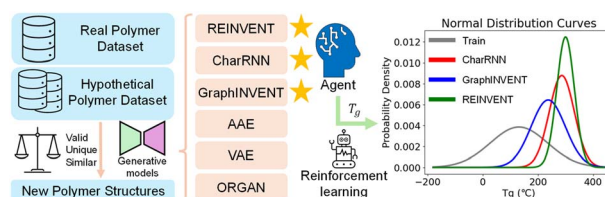


PAPERS

910

Benchmarking study of deep generative models for inverse polymer design

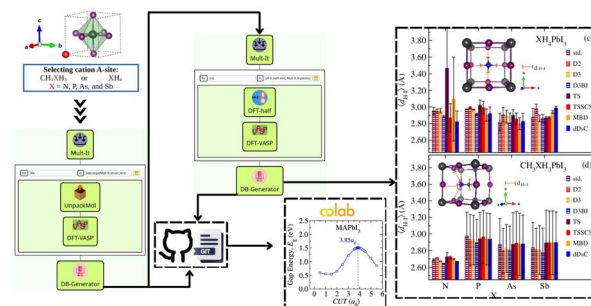
Tianle Yue, Lei Tao, Vikas Varshney and Ying Li*



927

Digital workflow optimization of van der Waals methods for improved halide perovskite solar materials

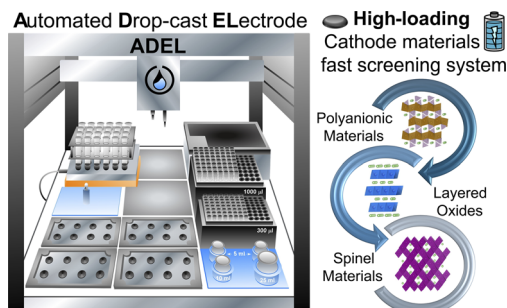
Celso R. C. Rêgo,* Wolfgang Wenzel, Maurício J. Piotrowski, Alexandre C. Dias, Carlos Maciel de Oliveira Bastos, Luis O. de Araujo and Diego Guedes-Sobrinho



943

ADEL: an automated drop-cast electrode setup for high-throughput screening of battery materials

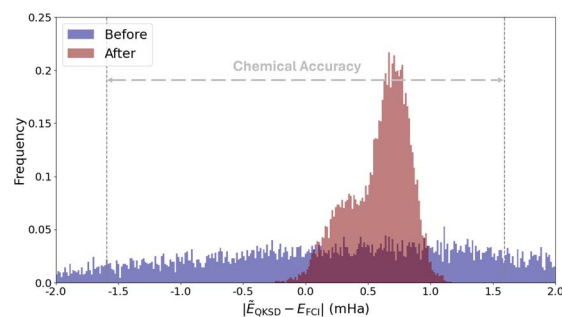
Maha Ismail, Maria Angeles Cabañero, Joseba Orive, Lakshmipriya Musuvadhi Babulal, Javier Garcia, Maria C. Morant-Miñana, Jean-Luc Dauvergne, Francisco Bonilla, Iciar Monterrubio, Javier Carrasco, Amaia Saracibar and Marine Reynaud*



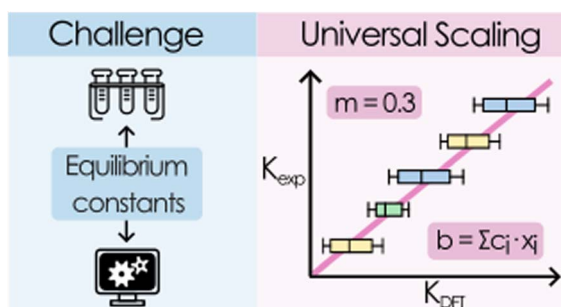
954

Efficient strategies for reducing sampling error in quantum Krylov subspace diagonalization

Gwonhak Lee, Seonghoon Choi, Joonsuk Huh* and Artur F. Izmaylov*



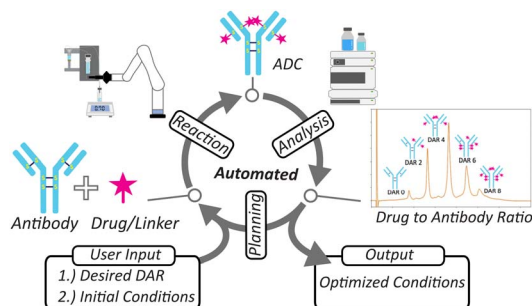
970



Towards a universal scaling method for predicting equilibrium constants of polyoxometalates

Jordi Buils, Diego Garay-Ruiz, Enric Petrus,*
Mireia Segado-Centellas and Carles Bo*

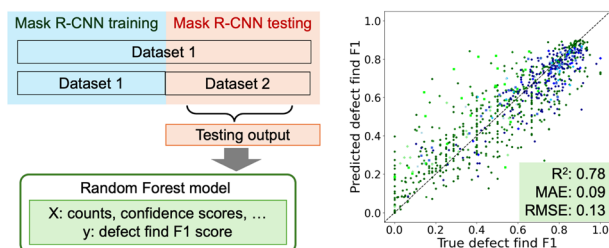
979



Automating stochastic antibody–drug conjugation: a self-driving lab approach for enhanced therapeutic development

Liam Roberts, Matthew E. Reish, Jerrica Yang,
Wenyu Zhang, Joshua S. Derasp* and Jason E. Hein*

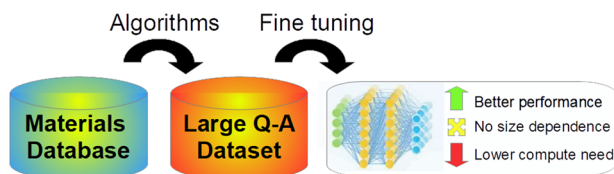
987



Predicting performance of object detection models in electron microscopy using random forests

Ni Li, Ryan Jacobs, Matthew Lynch, Vedit Agrawal,
Kevin Field and Dane Morgan*

998



Auto-generating question-answering datasets with domain-specific knowledge for language models in scientific tasks

Zongqian Li and Jacqueline M. Cole*

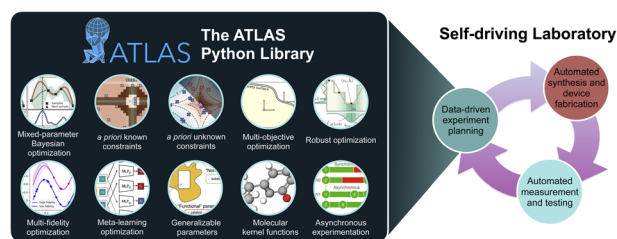


PAPERS

1006

Atlas: a brain for self-driving laboratories

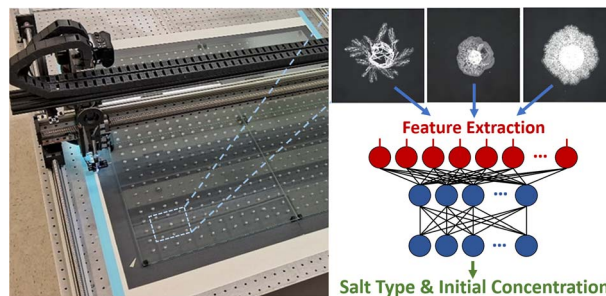
Riley J. Hickman,^{*} Malcolm Sim, Sergio Pablo-García, Gary Tom, Ivan Woolhouse, Han Hao, Zeqing Bao, Pauric Bannigan, Christine Allen, Matteo Aldeghi and Alán Aspuru-Guzik



1030

High-throughput robotic collection, imaging, and machine learning analysis of salt patterns: composition and concentration from dried droplet photos

Bruno C. Batista, Amrutha S. V., Jie Yan, Beni B. Dangi and Oliver Steinbock^{*}



1042

BitBIRCH: efficient clustering of large molecular libraries

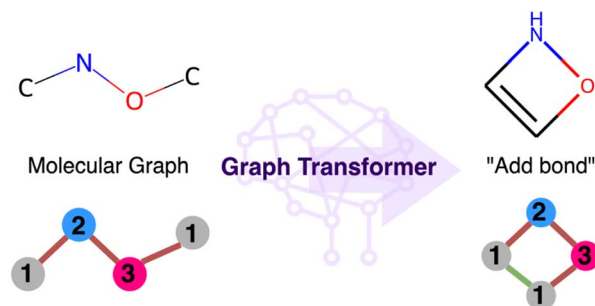
Kenneth López Pérez, Vicky Jung, Lexin Chen, Kate Huddleston and Ramón Alain Miranda-Quintana^{*}



1052

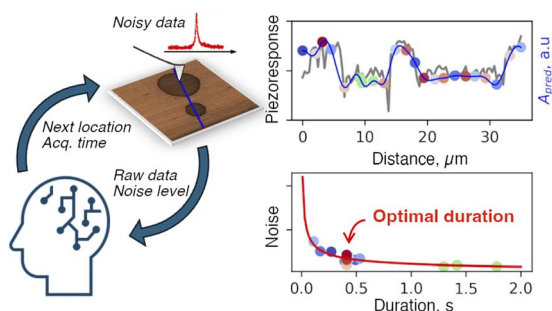
GraphXForm: graph transformer for computer-aided molecular design

Jonathan Pirnay, Jan G. Rittig, Alexander B. Wolf, Martin Grohe, Jakob Burger, Alexander Mitsos and Dominik G. Grimm^{*}



PAPERS

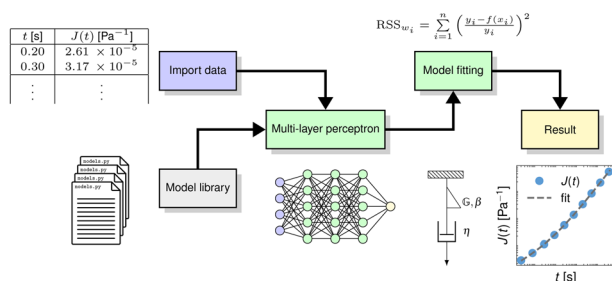
1066



Measurements with noise: Bayesian optimization for co-optimizing noise and property discovery in automated experiments

Boris N. Slautin,^{*} Yu Liu, Jan Dec, Vladimir V. Shvartsman, Doru C. Lupascu, Maxim A. Ziatdinov and Sergei V. Kalinin^{*}

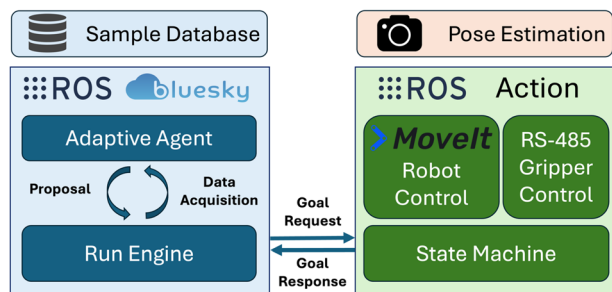
1075



pyRheo: an open-source Python package for complex rheology

Isaac Y. Miranda-Valdez,^{*} Aaro Niinistö, Tero Mäkinen, Juha Lejon, Juha Koivisto and Mikko J. Alava

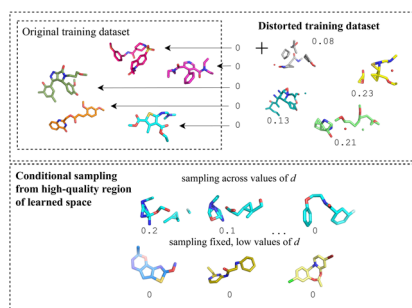
1083



Robotic integration for end-stations at scientific user facilities

Chandima Fernando, Hailey Marcello, Jakub Wlodek, John Sinsheimer, Daniel Olds, Stuart I. Campbell and Phillip M. Maffettone^{*}

1092



Improving structural plausibility in diffusion-based 3D molecule generation via property-conditioned training with distorted molecules

Lucy Vost, Vijil Chenthamarakshan, Payel Das and Charlotte M. Deane^{*}



1100

Ligand design for ^{227}Ac extraction by active learning and molecular topology

Jeffrey A. Laub and Konstantinos D. Vogiatzis*

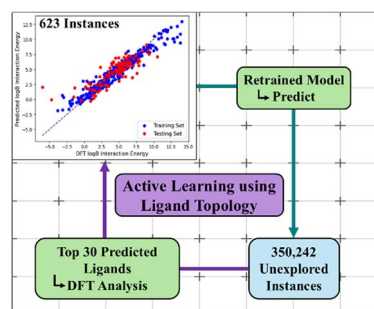


Fig. 1

Open Access Article. Published on 09 April 2025. Downloaded on 26/08/2025 18:33:29.

This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

