

# Digital Discovery

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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

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### Digital discovery and the new experimental frontier

S. Hessam M. Mehr

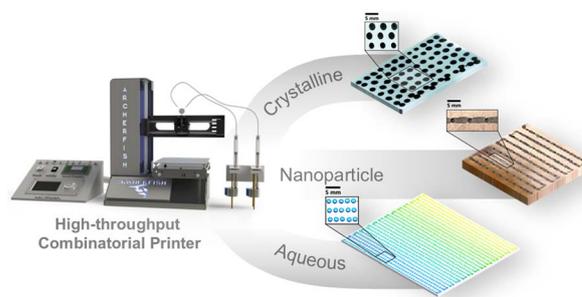


## PAPERS

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### 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\*



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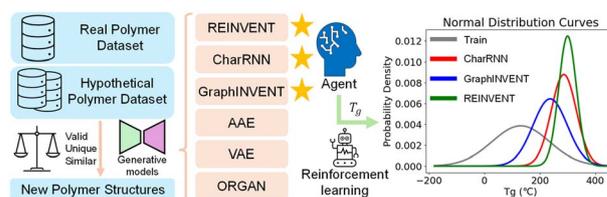
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## Benchmarking study of deep generative models for inverse polymer design

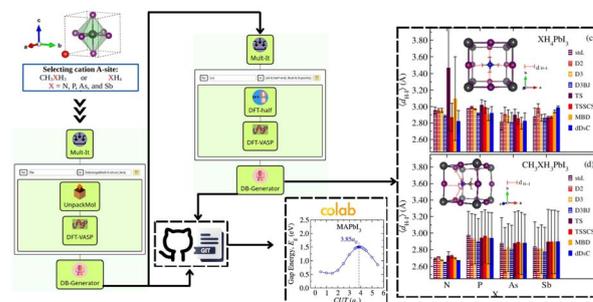
Tianle Yue, Lei Tao, Vikas Varshney and Ying Li\*



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

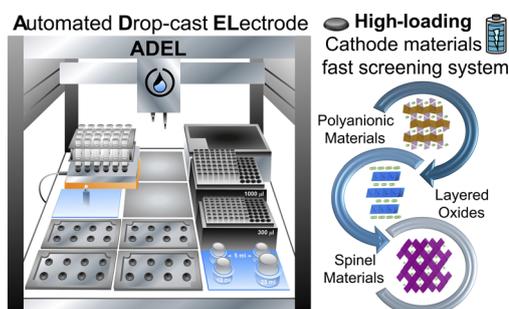
Celso R. C. Rêgo,\* Wolfgang Wenzel, Maurício J. Piotrowski, Alexandre C. Dias, Carlos Maciel de Oliveira Bastos, Luis O. de Araujo and Diego Guedes-Sobrinho



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

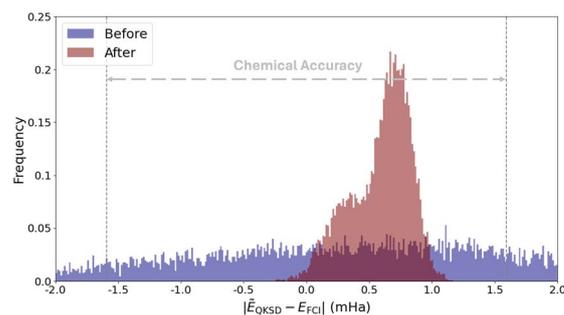
Maha Ismail, Maria Angeles Cabañero, Joseba Orive, Lakshmi Priya Musuvadhi Babulal, Javier Garcia, Maria C. Morant-Miñana, Jean-Luc Dauvergne, Francisco Bonilla, Iciar Monterrubio, Javier Carrasco, Amaia Saracibar and Marine Reynaud\*



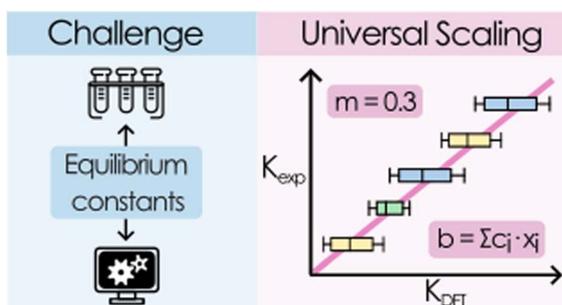
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## Efficient strategies for reducing sampling error in quantum Krylov subspace diagonalization

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



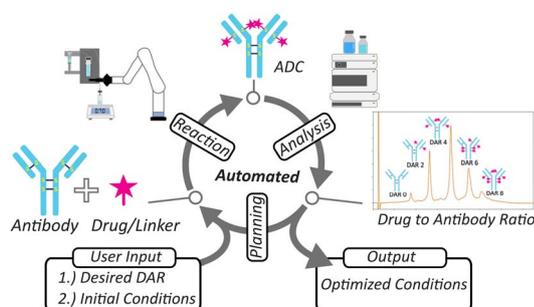
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### Towards a universal scaling method for predicting equilibrium constants of polyoxometalates

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

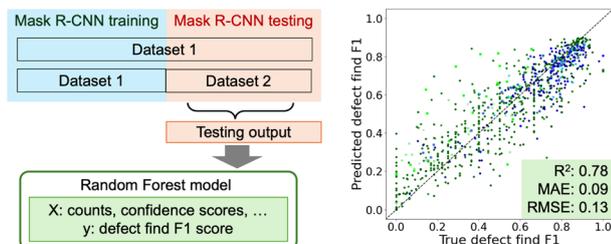
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### Automating stochastic antibody–drug conjugation: a self-driving lab approach for enhanced therapeutic development

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

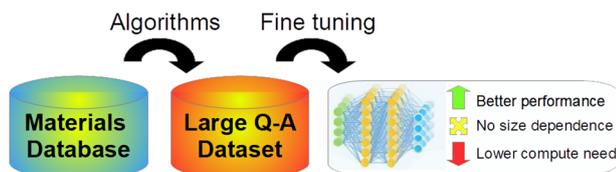
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### Predicting performance of object detection models in electron microscopy using random forests

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

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

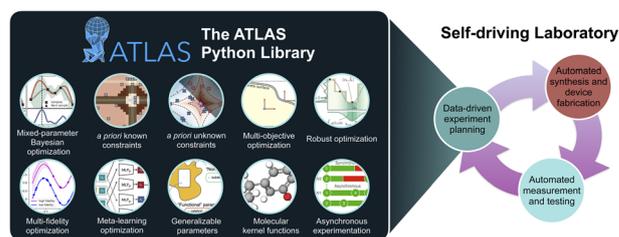
Zongqian Li and Jacqueline M. Cole\*



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**Atlas: a brain for self-driving laboratories**

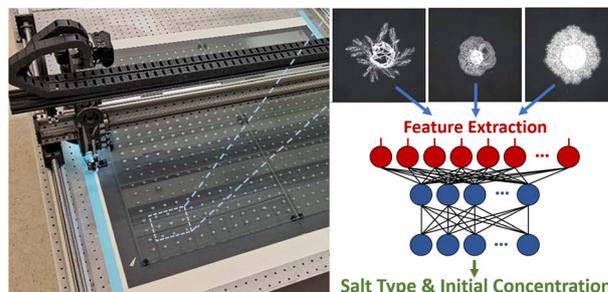
Riley J. Hickman,\* Malcolm Sim, Sergio Pablo-García, Gary Tom, Ivan Woolhouse, Han Hao, Zeqing Bao, Pauric Bannigan, Christine Allen, Matteo Aldeghi and Alán Aspuru-Guzik



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**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\*



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**BitBIRCH: efficient clustering of large molecular libraries**

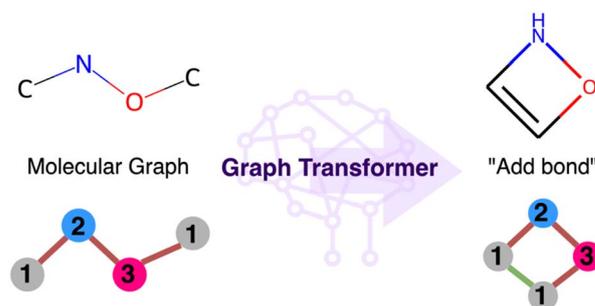
Kenneth López Pérez, Vicky Jung, Lexin Chen, Kate Huddleston and Ramón Alain Miranda-Quintana\*



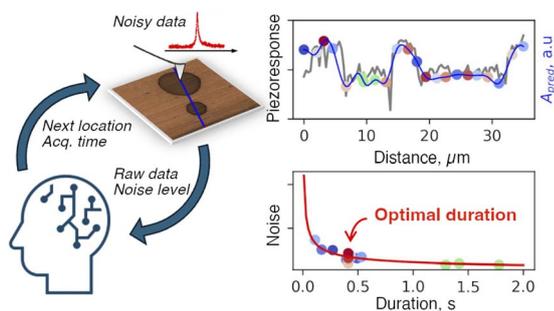
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**GraphXForm: graph transformer for computer-aided molecular design**

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



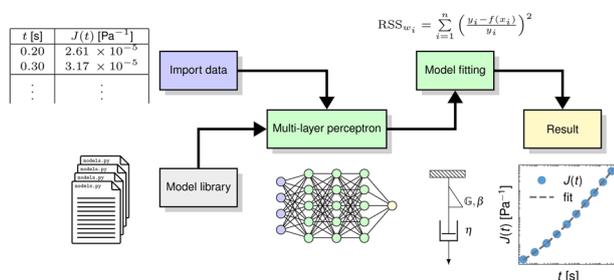
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### Measurements with noise: Bayesian optimization for co-optimizing noise and property discovery in automated experiments

Boris N. Slautin,<sup>\*</sup> Yu Liu, Jan Dec, Vladimir V. Shvartsman, Doru C. Lupascu, Maxim A. Ziatdinov and Sergei V. Kalinin<sup>\*</sup>

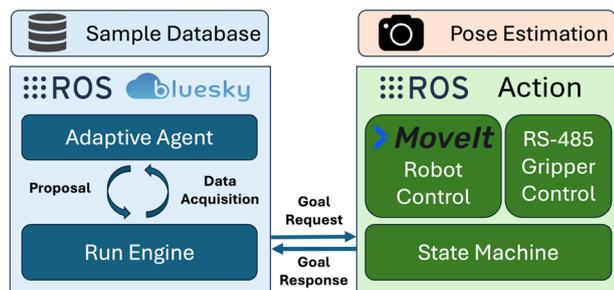
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### pyRheo: an open-source Python package for complex rheology

Isaac Y. Miranda-Valdez,<sup>\*</sup> Aaro Niinistö, Tero Mäkinen, Juha Lejon, Juha Koivisto and Mikko J. Alava

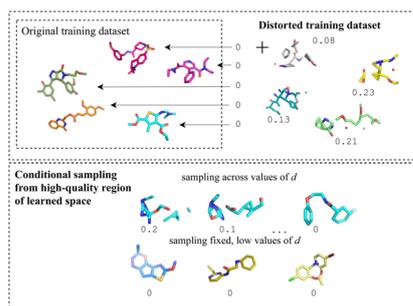
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### Robotic integration for end-stations at scientific user facilities

Chandima Fernando, Hailey Marcello, Jakub Wlodek, John Sinshemer, Daniel Olds, Stuart I. Campbell and Phillip M. Maffettone<sup>\*</sup>

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### 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<sup>\*</sup>



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## Ligand design for $^{227}\text{Ac}$ extraction by active learning and molecular topology

Jeffrey A. Laub and Konstantinos D. Vogiatzis\*

