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**Cover**
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**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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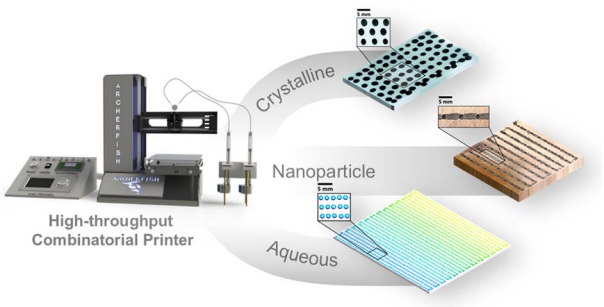

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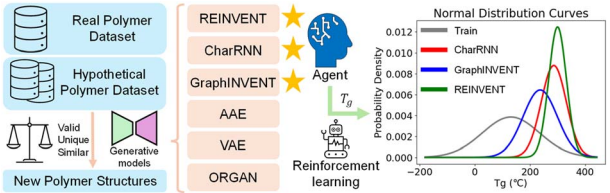




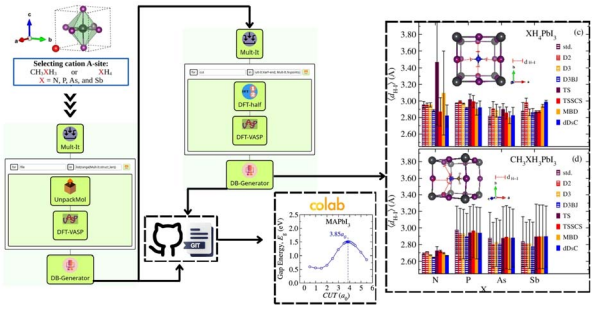




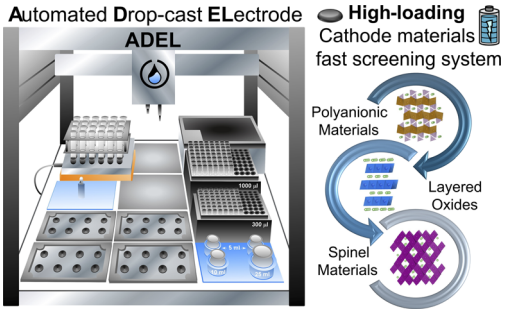




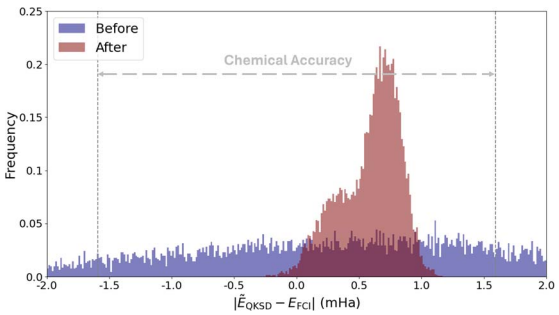

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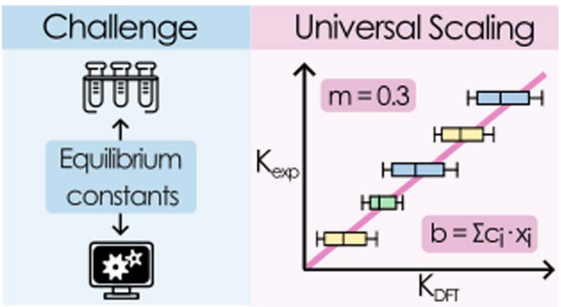


## Towards a universal scaling method for predicting equilibrium constants of polyoxometalates

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

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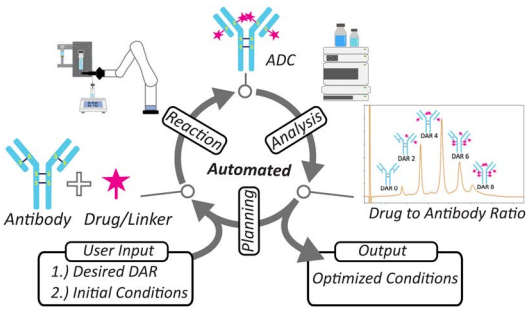


## Automating stochastic antibody–drug conjugation: a self-driving lab approach for enhanced therapeutic development

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

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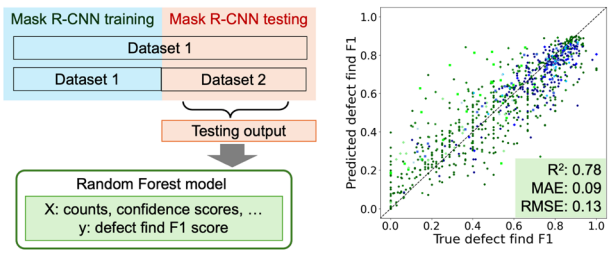


## Predicting performance of object detection models in electron microscopy using random forests

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

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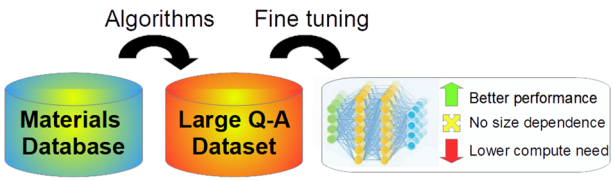


## Auto-generating question-answering datasets with domain-specific knowledge for language models in scientific tasks

Zongqian Li and Jacqueline M. Cole*

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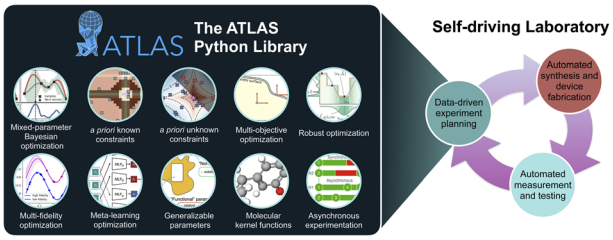




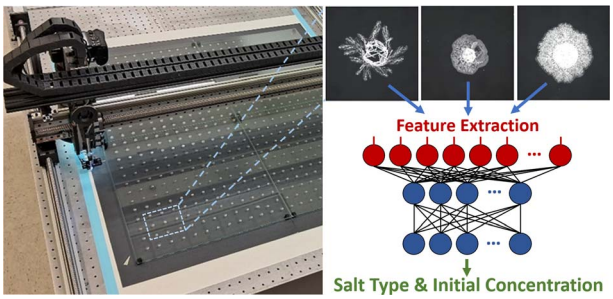




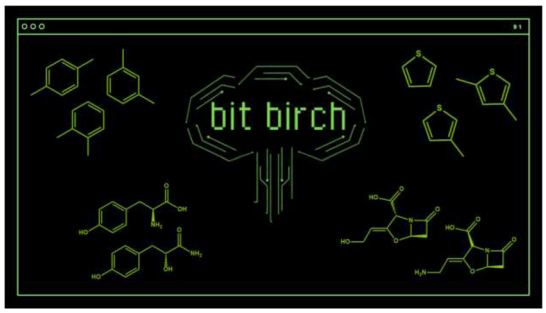




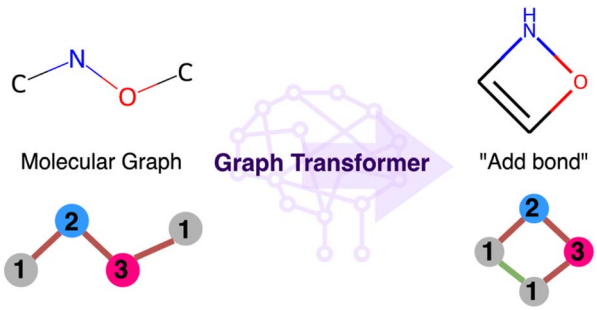

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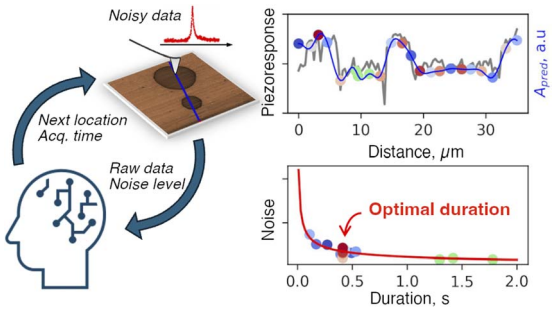


## Measurements with noise: Bayesian optimization for co-optimizing noise and property discovery in automated experiments

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

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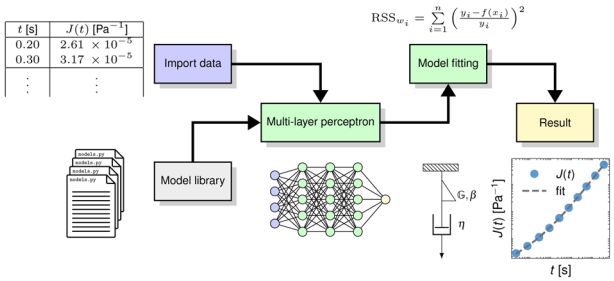


## pyRheo: an open-source Python package for complex rheology

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

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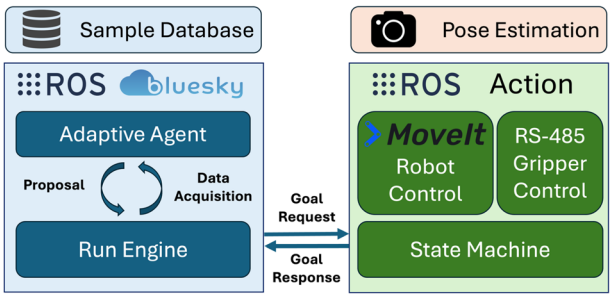


## Robotic integration for end-stations at scientific user facilities

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

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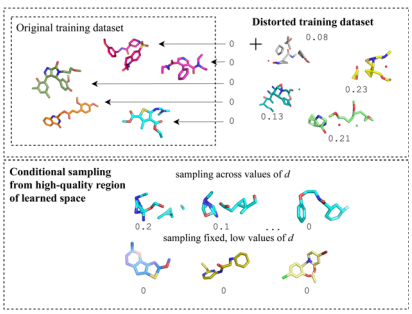


## Improving structural plausibility in diffusion-based 3D molecule generation *via* property-conditioned training with distorted molecules

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

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

Jeffrey A. Laub and Konstantinos D. Vogiatzis*