

# Digital Discovery

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**Inside cover**  
See Shu Huang and Jacqueline M. Cole, pp. 1710–1720. Image reproduced by permission of Shu Huang and Nan Tian, who used imagery from rawpixel.com from Freepik, from *Digital Discovery*, 2023, 2, 1710.

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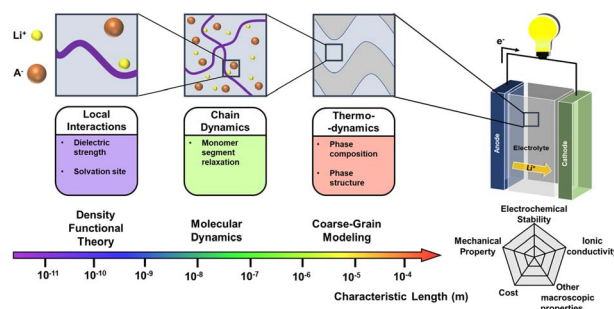


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1660

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Kaiyang Wang, Haoyuan Shi, Tianjiao Li, Liming Zhao, Hanfeng Zhai, Deepa Korani and Jingjie Yeo\*



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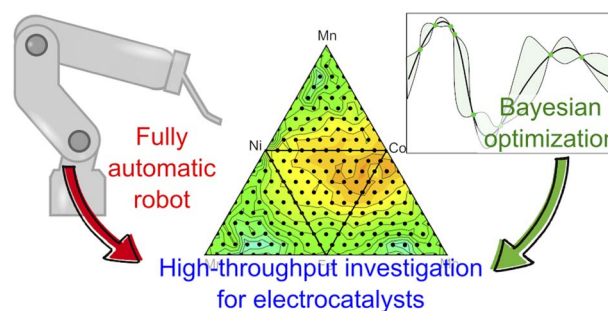


## COMMUNICATIONS

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**An automatic robot system for machine learning–assisted high-throughput screening of composite electrocatalysts**

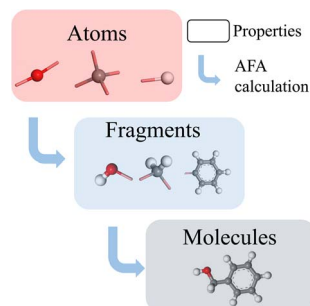
Masanori Kodera\* and Kazuhiro Sayama\*



1688

**Atomic fragment approximation from a tensor network**

Haoxiang Lin and Xi Zhu\*

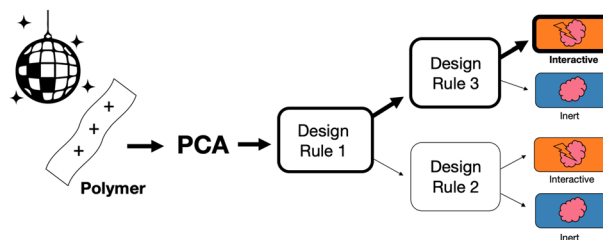


## PAPERS

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**An interpretable machine learning framework for modelling macromolecular interaction mechanisms with nuclear magnetic resonance**

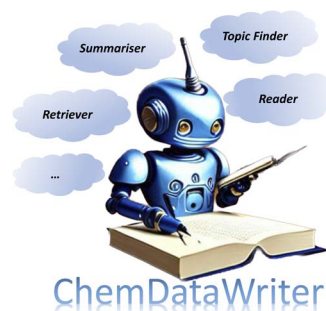
Samantha Stuart, Jeffrey Watchorn and Frank X. Gu\*



1710

**ChemDataWriter: a transformer-based toolkit for auto-generating books that summarise research**

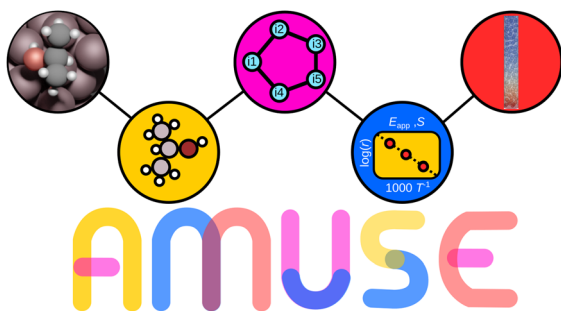
Shu Huang and Jacqueline M. Cole\*



ChemDataWriter



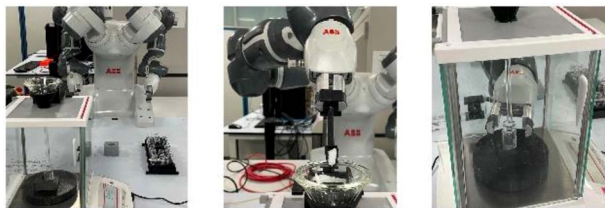
1721



### Automated MULTiscale simulation environment

Albert Sabadell-Rendón,<sup>\*</sup> Kamila Kaźmierczak, Santiago Morandi, Florian Euzenat, Daniel Curulla-Ferré and Núria López<sup>\*</sup>

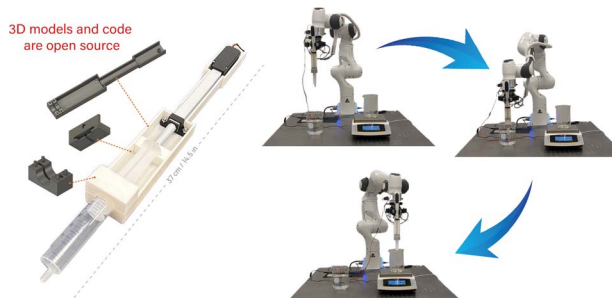
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### Autonomous biomimetic solid dispensing using a dual-arm robotic manipulator

Ying Jiang, Hatem Fakhruddin, Gabriella Pizzuto, Louis Longley, Ai He, Tianwei Dai, Rob Clowes, Nicola Rankin and Andrew I. Cooper<sup>\*</sup>

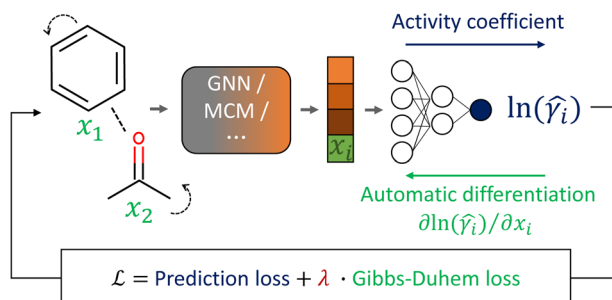
1745



### Digital pipette: open hardware for liquid transfer in self-driving laboratories

Naruki Yoshikawa,<sup>\*</sup> Kourosh Darvish, Mohammad Ghazi Vakili, Animesh Garg<sup>\*</sup> and Alán Aspuru-Guzik<sup>\*</sup>

1752



### Gibbs–Duhem-informed neural networks for binary activity coefficient prediction

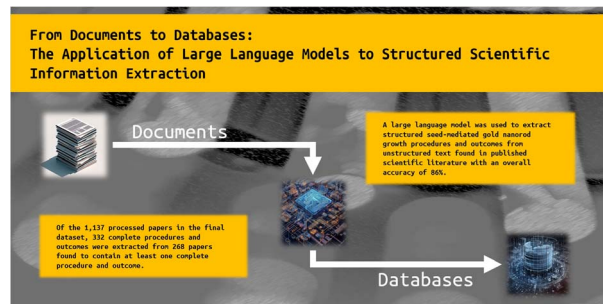
Jan G. Rittig, Kobi C. Felton, Alexei A. Lapkin and Alexander Mitsos<sup>\*</sup>



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## Extracting structured seed-mediated gold nanorod growth procedures from scientific text with LLMs

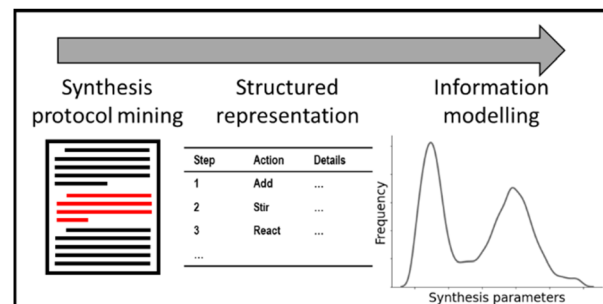
Nicholas Walker,<sup>\*</sup> Sanghoon Lee, John Dagdelen, Kevin Cruse, Samuel Gleason, Alexander Dunn, Gerbrand Ceder, A. Paul Alivisatos, Kristin A. Persson and Anubhav Jain<sup>\*</sup>



1783

## Unveiling the synthesis patterns of nanomaterials: a text mining and meta-analysis approach with ZIF-8 as a case study

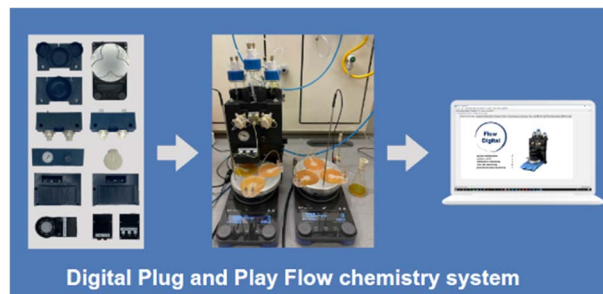
Joseph R. H. Manning<sup>\*</sup> and Lev Sarkisov<sup>\*</sup>



1797

## Digitisation of a modular plug and play 3D printed continuous flow system for chemical synthesis

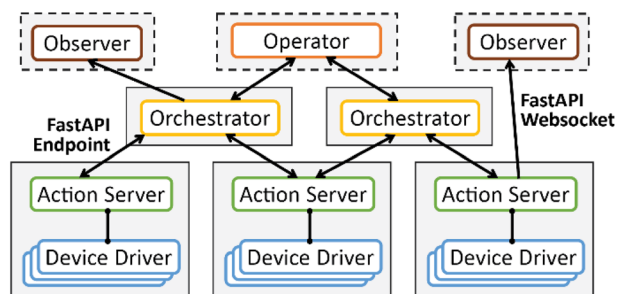
Mireia Benito Montaner, Matthew R. Penny and Stephen T. Hilton<sup>\*</sup>



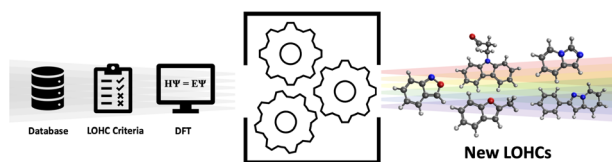
1806

## Orchestrating nimble experiments across interconnected labs

Dan Guevarra,<sup>\*</sup> Kevin Kan, Yungchieh Lai, Ryan J. R. Jones, Lan Zhou, Phillip Donnelly, Matthias Richter, Helge S. Stein and John M. Gregoire<sup>\*</sup>



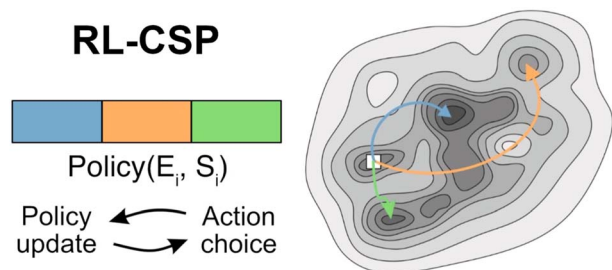
1813



### Uncovering novel liquid organic hydrogen carriers: a systematic exploration of chemical compound space using cheminformatics and quantum chemical methods

Hassan Harb, Sarah N. Elliott, Logan Ward, Ian T. Foster, Stephen J. Klippenstein, Larry A. Curtiss and Rajeev Surendran Assary\*

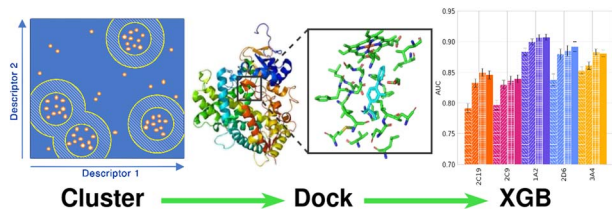
1831



### Reinforcement learning in crystal structure prediction

Elena Zamaraeva, Christopher M. Collins, Dmytro Antypov, Vladimir V. Gusev, Rahul Savani,\* Matthew S. Dyer, George R. Darling, Igor Potapov, Matthew J. Rosseinsky\* and Paul G. Spirakis

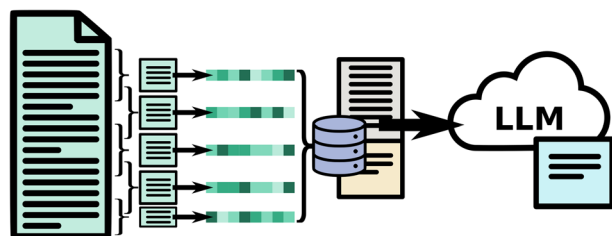
1841



### Machine learning-augmented docking. 1. CYP inhibition prediction

Benjamin Weiser,\* Jérôme Genzling, Mihai Burai-Patrascu, Ophélie Rostaing and Nicolas Moitessier\*

1850



### Domain-specific chatbots for science using embeddings

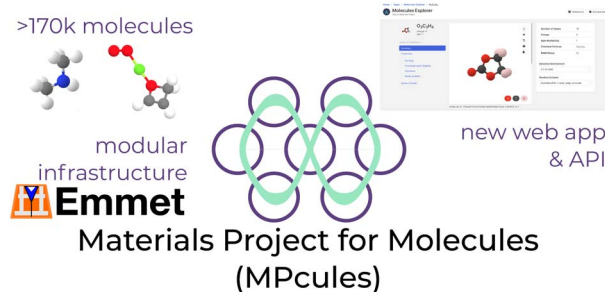
Kevin G. Yager\*



1862

## A database of molecular properties integrated in the Materials Project

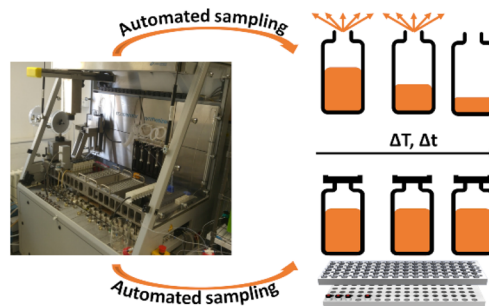
Evan Walter Clark Spotte-Smith,<sup>\*</sup> Orion Archer Cohen, Samuel M. Blau, Jason M. Munro, Ruoxi Yang, Rishabh D. Guha, Hetal D. Patel, Sudarshan Vijay, Patrick Huck, Ryan Kingsbury, Matthew K. Horton and Kristin A. Persson<sup>\*</sup>



1883

## Best practice for sampling in automated parallel synthesizers

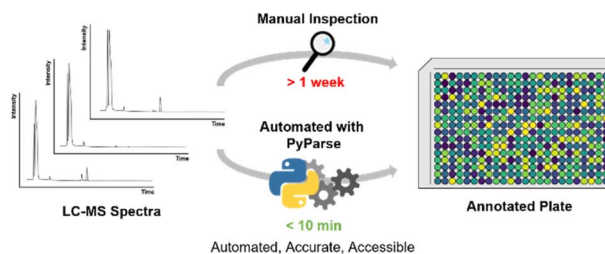
Michael Ringleb, Timo Schuett, Stefan Zechel and Ulrich S. Schubert<sup>\*</sup>



1894

## Automated LC-MS analysis and data extraction for high-throughput chemistry

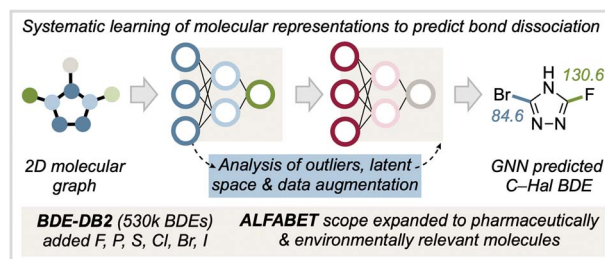
Joseph Mason,<sup>\*</sup> Harry Wilders, David J. Fallon, Ross P. Thomas, Jacob T. Bush, Nicholas C. O. Tomkinson and Francesco Rianjongdee



1900

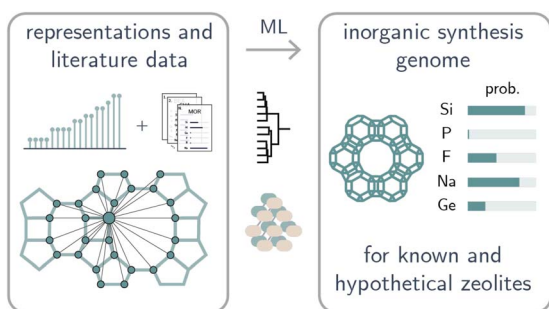
## Expansion of bond dissociation prediction with machine learning to medicinally and environmentally relevant chemical space

Shree Sowndarya S. V., Yeonjoon Kim, Seonah Kim,<sup>\*</sup> Peter C. St. John<sup>\*</sup> and Robert S. Paton<sup>\*</sup>



## PAPERS

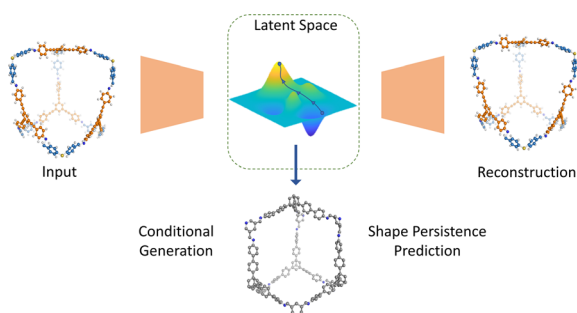
1911



### Inorganic synthesis-structure maps in zeolites with machine learning and crystallographic distances

Daniel Schwalbe-Koda,\* Daniel E. Widdowson, Tuan Anh Pham and Vitaliy A. Kurlin\*

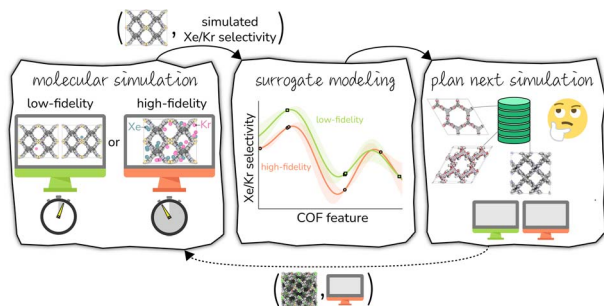
1925



### Deep generative design of porous organic cages via a variational autoencoder

Jiajun Zhou, Austin Mroz and Kim E. Jelfs\*

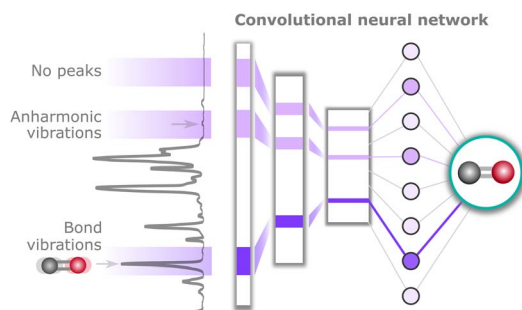
1937



### Multi-fidelity Bayesian optimization of covalent organic frameworks for xenon/krypton separations

Nickolas Gantzer, Aryan Deshwal, Janardhan Rao Doppa\* and Cory M. Simon\*

1957



### Understanding the patterns that neural networks learn from chemical spectra

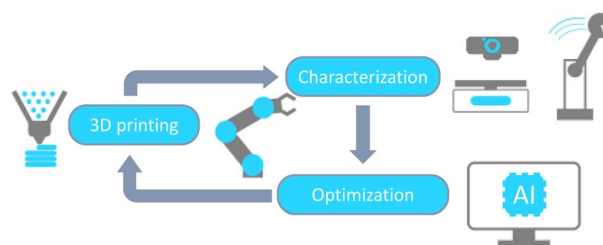
Laura Hannemose Rieger, Max Wilson, Tejs Vegge and Eibar Flores\*



1969

### Robotically automated 3D printing and testing of thermoplastic material specimens

Miguel Hernández-del-Valle, Christina Schenk, Lucía Echevarría-Pastrana, Burcu Ozdemir, Enrique Dios-Lázaro, Jorge Ilarraza-Zuazo, De-Yi Wang and Maciej Haranczyk\*



1980

### Towards a modular architecture for science factories

Rafael Vescovi, Tobias Ginsburg, Kyle Hippe, Doga Ozgulbas, Casey Stone, Abraham Stroka, Rory Butler, Ben Blaiszik, Tom Brettin, Kyle Chard, Mark Hereld, Arvind Ramanathan, Rick Stevens, Aikaterini Vriza, Jie Xu, Qingteng Zhang and Ian Foster\*

