

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.

PERSPECTIVE

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What is missing in autonomous discovery: open challenges for the community

Phillip M. Maffettone,* Pascal Friederich,* Sterling G. Baird, Ben Blaiszik, Keith A. Brown, Stuart I. Campbell, Orion A. Cohen, Rebecca L. Davis, Ian T. Foster, Navid Haghmoradi, Mark Hereld, Howie Jores, Nicole Jung, Ha-Kyung Kwon, Gabriella Pizzuto, Jacob Rintamaki, Casper Steinmann, Luca Torresi and Shijing Sun

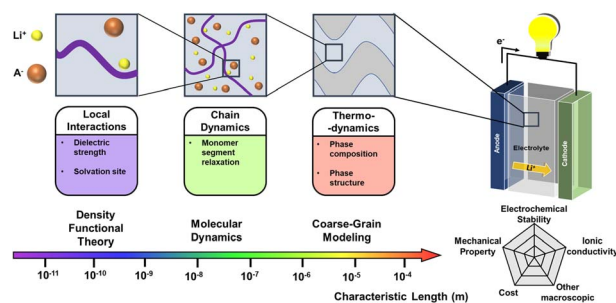


REVIEW

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Computational and data-driven modelling of solid polymer electrolytes

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



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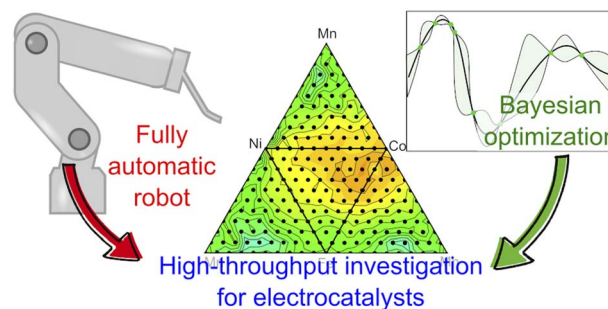


COMMUNICATIONS

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

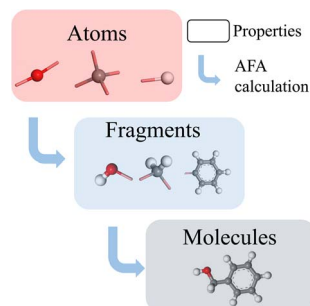
Masanori Kodera* and Kazuhiro Sayama*



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Atomic fragment approximation from a tensor network

Haoxiang Lin and Xi Zhu*

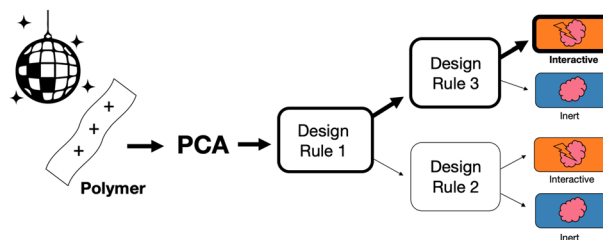


PAPERS

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

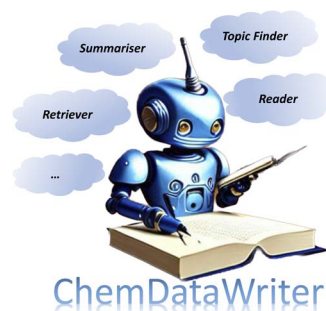
Samantha Stuart, Jeffrey Watchorn and Frank X. Gu*



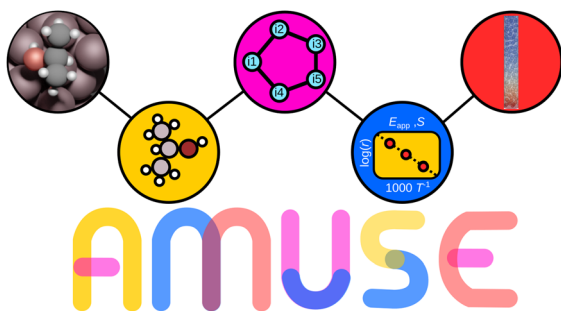
1710

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

Shu Huang and Jacqueline M. Cole*



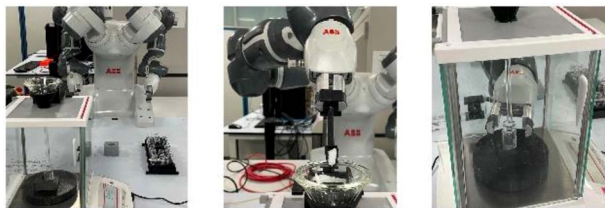
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Automated MULTiscale simulation environment

Albert Sabadell-Rendón,^{*} Kamila Kaźmierczak, Santiago Morandi, Florian Euzenat, Daniel Curulla-Ferré and Núria López^{*}

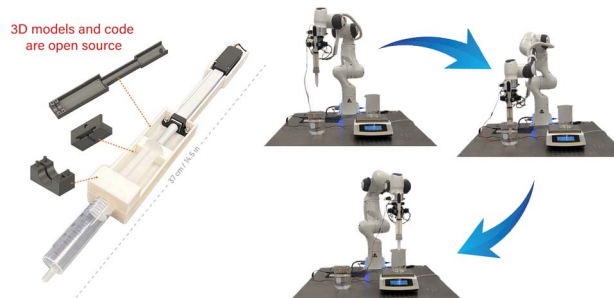
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Autonomous biomimetic solid dispensing using a dual-arm robotic manipulator

Ying Jiang, Hatem Fakhruddin, Gabriella Pizzuto, Louis Longley, Ai He, Tianwei Dai, Rob Clowes, Nicola Rankin and Andrew I. Cooper^{*}

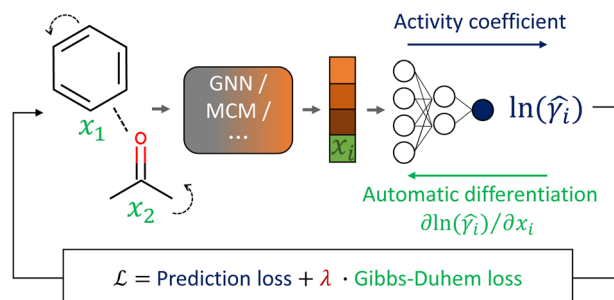
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Digital pipette: open hardware for liquid transfer in self-driving laboratories

Naruki Yoshikawa,^{*} Kourosh Darvish, Mohammad Ghazi Vakili, Animesh Garg^{*} and Alán Aspuru-Guzik^{*}

1752



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

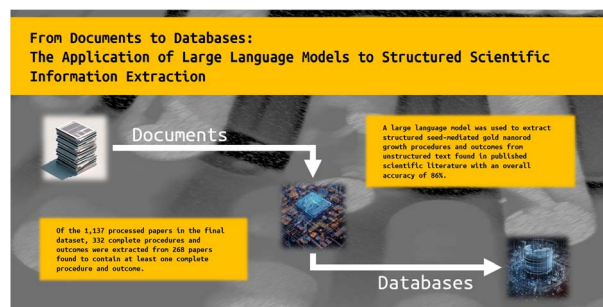
Jan G. Rittig, Kobi C. Felton, Alexei A. Lapkin and Alexander Mitsos^{*}



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

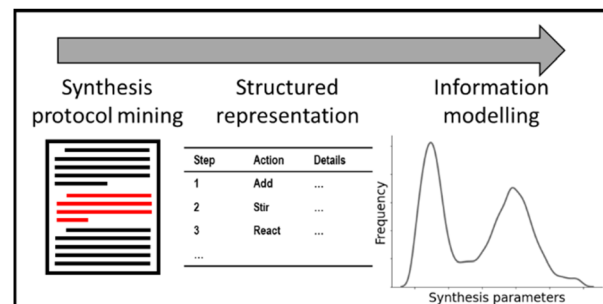
Nicholas Walker,* Sanghoon Lee, John Dagdelen, Kevin Cruse, Samuel Gleason, Alexander Dunn, Gerbrand Ceder, A. Paul Alivisatos, Kristin A. Persson and Anubhav Jain*



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

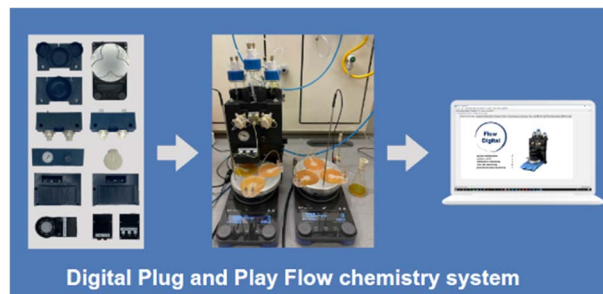
Joseph R. H. Manning* and Lev Sarkisov*



1797

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

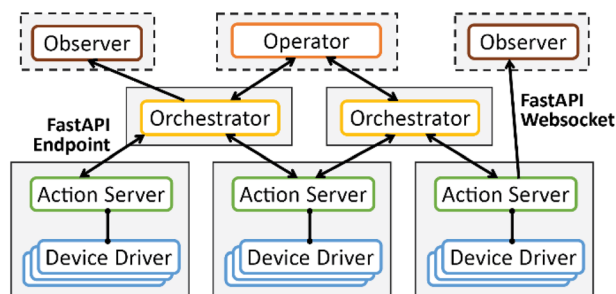
Mireia Benito Montaner, Matthew R. Penny and Stephen T. Hilton*



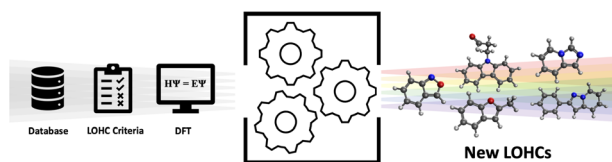
1806

Orchestrating nimble experiments across interconnected labs

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



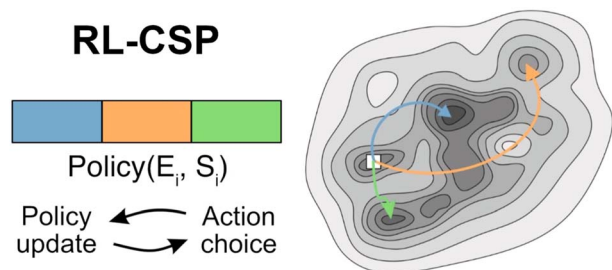
1813



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*

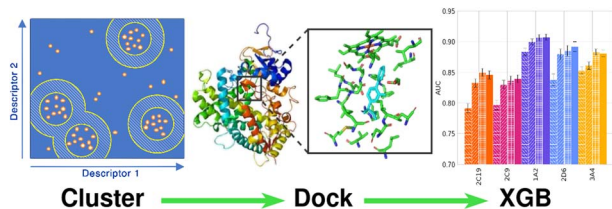
1831



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

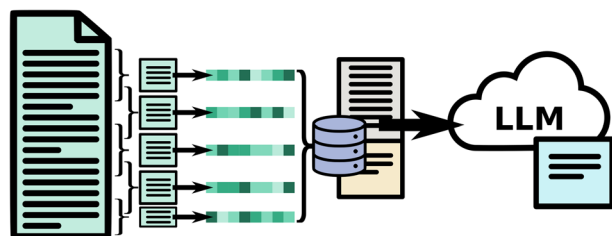
1841



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

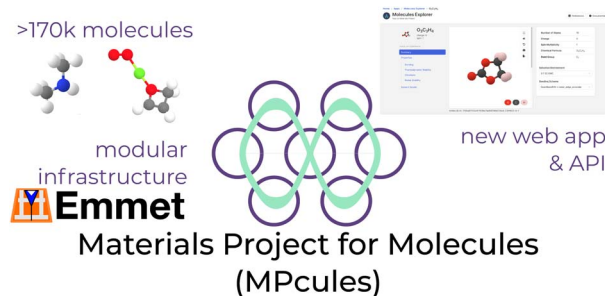
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A database of molecular properties integrated in the Materials Project

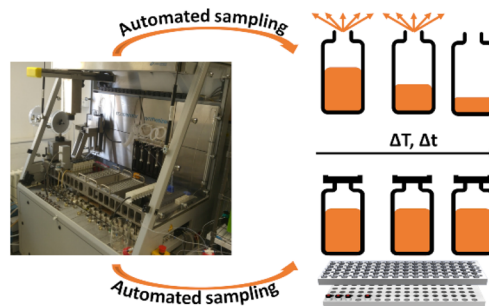
Evan Walter Clark Spotte-Smith,^{*} Orion Archer Cohen, Samuel M. Blau, Jason M. Munro, Ruoxi Yang, Rishabh D. Guha, Hetal D. Patel, Sudarshan Vijay, Patrick Huck, Ryan Kingsbury, Matthew K. Horton and Kristin A. Persson^{*}



1883

Best practice for sampling in automated parallel synthesizers

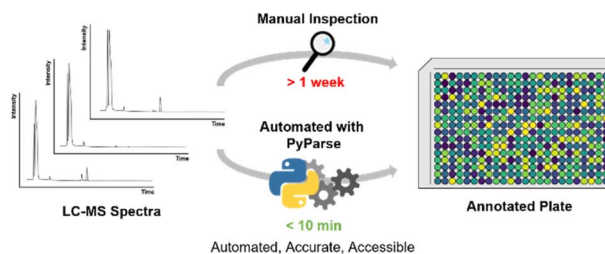
Michael Ringleb, Timo Schuett, Stefan Zechel and Ulrich S. Schubert^{*}



1894

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

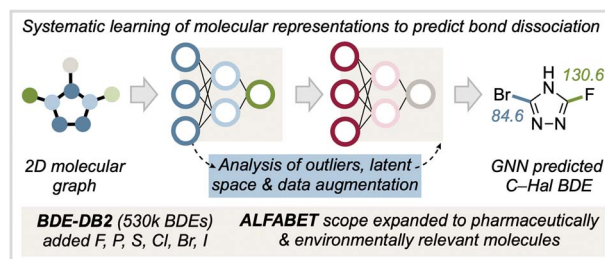
Joseph Mason,^{*} Harry Wilders, David J. Fallon, Ross P. Thomas, Jacob T. Bush, Nicholas C. O. Tomkinson and Francesco Rianjongdee



1900

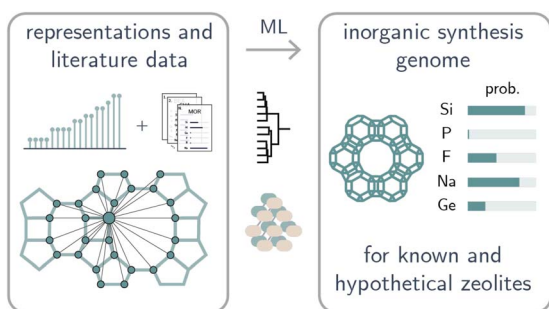
Expansion of bond dissociation prediction with machine learning to medicinally and environmentally relevant chemical space

Shree Sowndarya S. V., Yeonjoon Kim, Seonah Kim,^{*} Peter C. St. John^{*} and Robert S. Paton^{*}



PAPERS

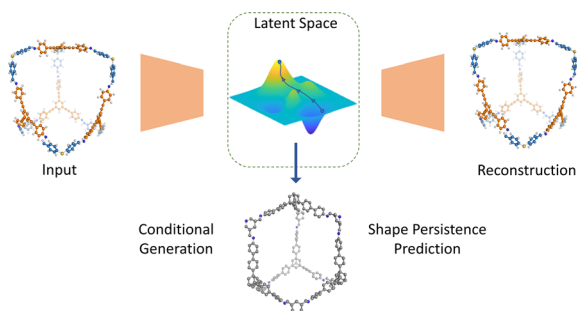
1911



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^{*}

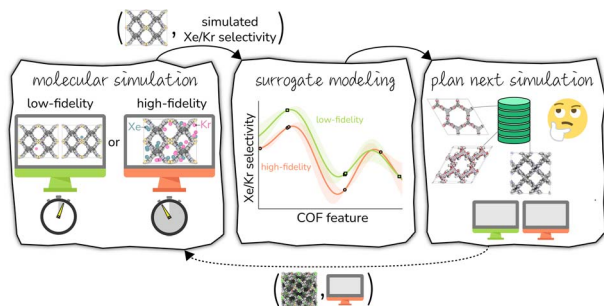
1925



Deep generative design of porous organic cages via a variational autoencoder

Jiajun Zhou, Austin Mroz and Kim E. Jelfs^{*}

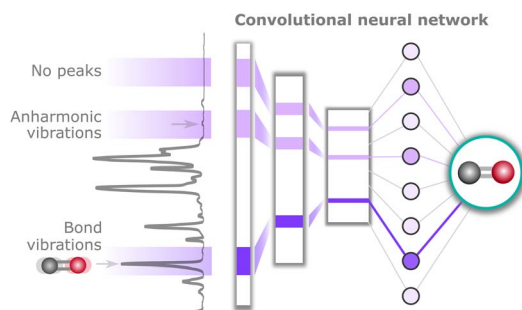
1937



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

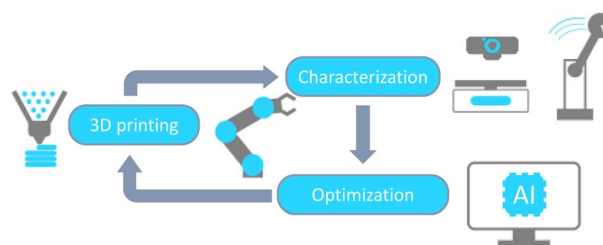
Laura Hannemose Rieger, Max Wilson, Tejs Vegge and Eibar Flores^{*}



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*

