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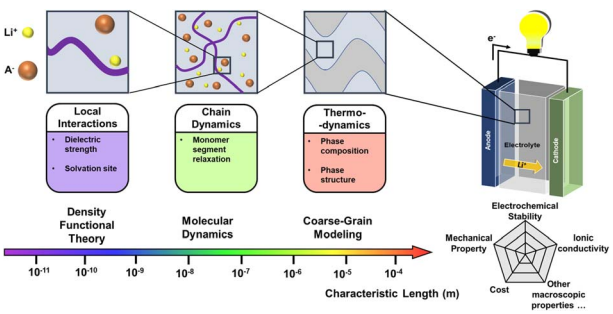
Inside cover
See Shu Huang and Jacqueline M. Cole, pp. 1710–1720. Image reproduced by permission of Shu Huang and Nan Tian, who used imagery from rawpixel.com from Freepik, from *Digital Discovery*, 2023, **2**, 1710.

PERSPECTIVE

REVIEW



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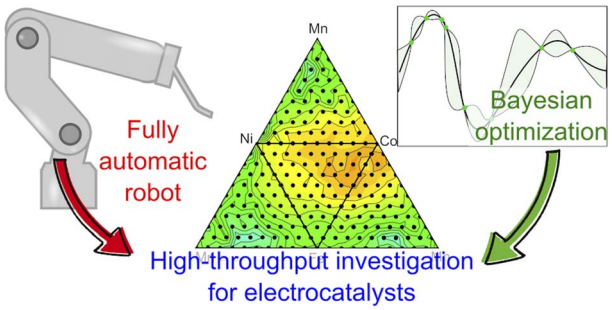

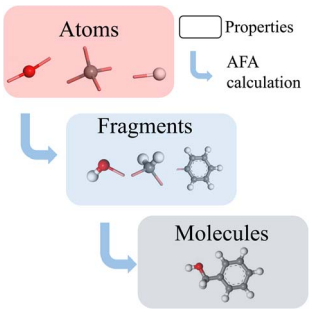

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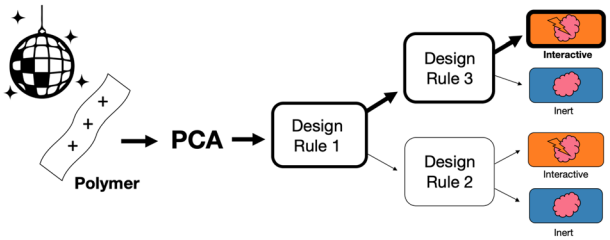

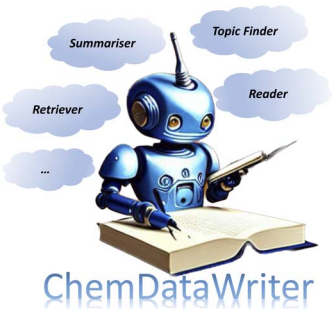

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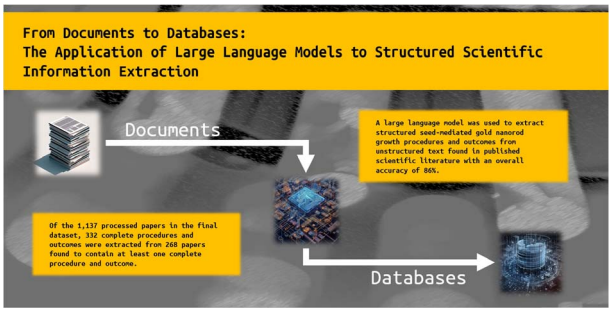

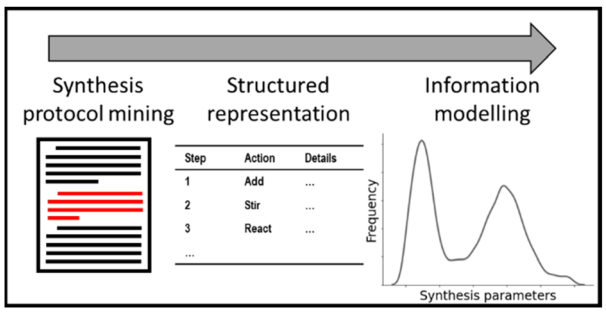

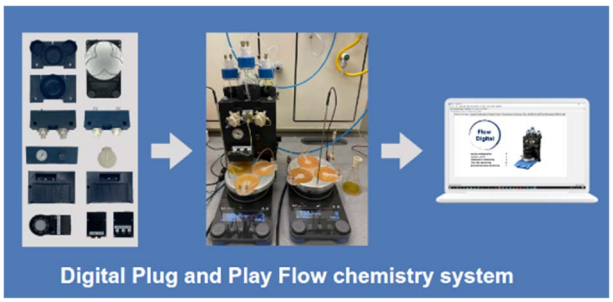

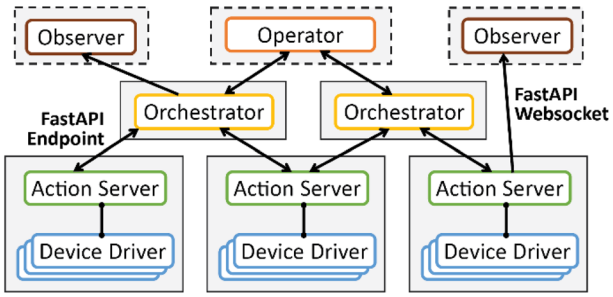

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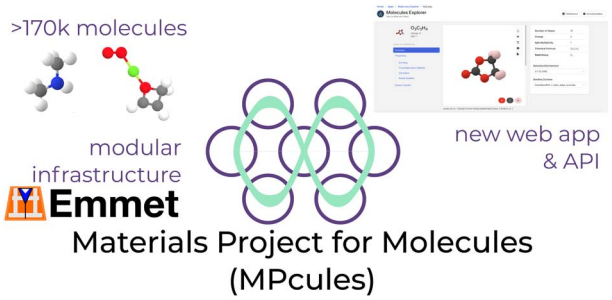
1862

A database of molecular properties integrated in the Materials Project

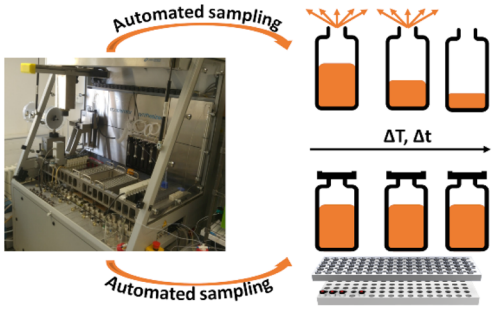
Evan Walter Clark Spotte-Smith,* Orion Archer Cohen, Samuel M. Blau, Jason M. Munro, Ruoxi Yang, Rishabh D. Guha, Hetal D. Patel, Sudarshan Vijay, Patrick Huck, Ryan Kingsbury, Matthew K. Horton and Kristin A. Persson*



1883

Best practice for sampling in automated parallel synthesizers

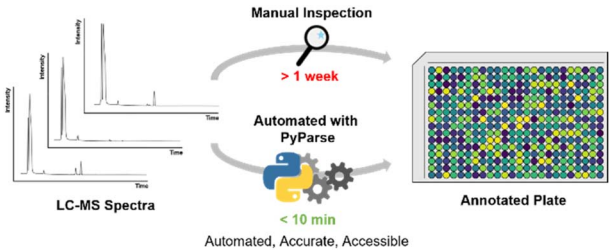
Michael Ringleb, Timo Schuett, Stefan Zechel and Ulrich S. Schubert*



1894

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

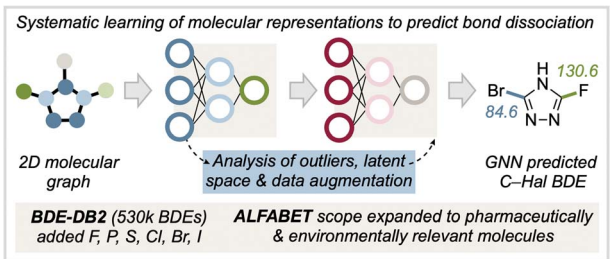
Joseph Mason,* Harry Wilders, David J. Fallon, Ross P. Thomas, Jacob T. Bush, Nicholas C. O. Tomkinson and Francesco Rianjongdee



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*



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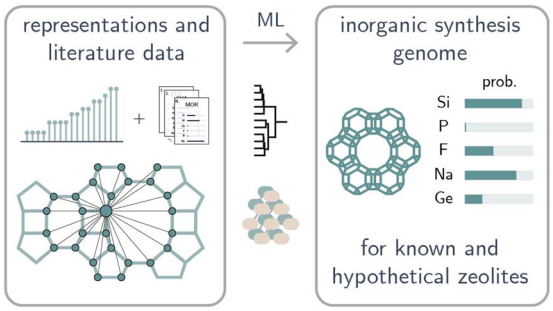
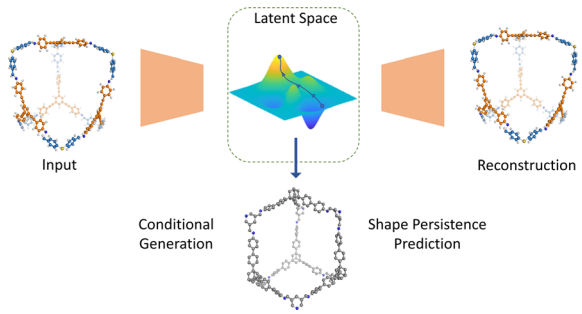
1911



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*

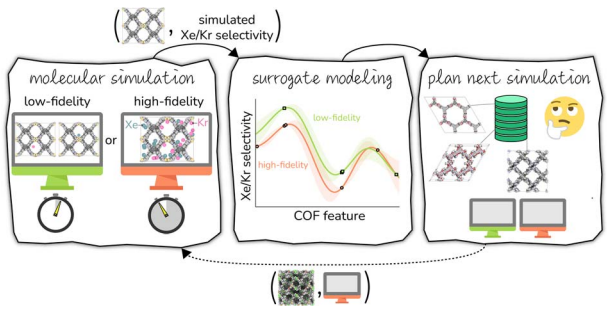
1925



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

Jiajun Zhou, Austin Mroz and Kim E. Jelfs*

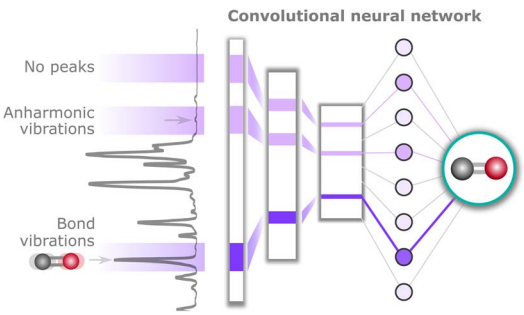
1937



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

Nickolas Gantzler, 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*

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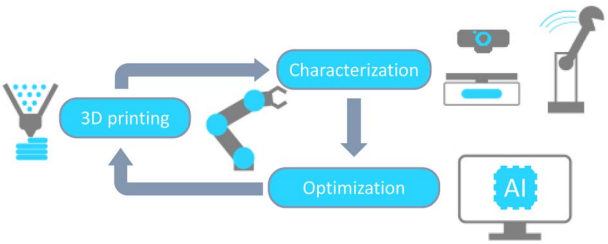
1969

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*