Digital Discovery

IN THIS ISSUE

Cover
See Wenbo Yang, Jinzhe Cao, Shengyang Tao *et al.*,
pp. 1958–1966. Image reproduced by permission of Wenbo Yang, Jinzhe Cao, and Shengyang Tao from *Digital Discovery*, 2024, **3**, 1958.

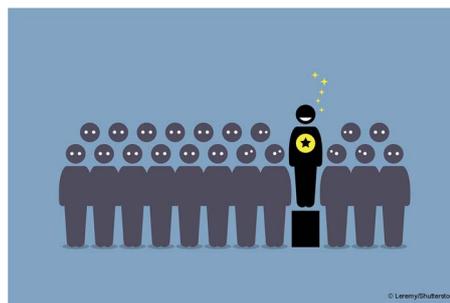**Inside cover**
See Stefan Bräse,
pp. 1923–1932. Image reproduced by permission of Stefan Bräse and Vincenzo Pani from *Digital Discovery*, 2024, **3**, 1923.

EDITORIAL

1922

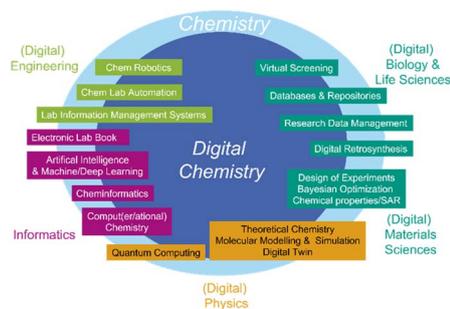**Outstanding Reviewers for *Digital Discovery* in 2023**

PERSPECTIVES

1923

Digital chemistry: navigating the confluence of computation and experimentation – definition, status quo, and future perspective

Stefan Bräse*

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**Fundamental questions
Elemental answers**

PERSPECTIVES

1933

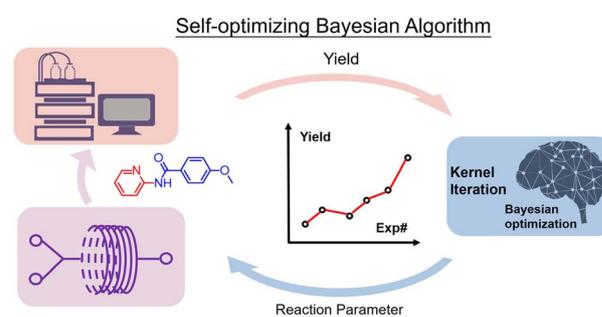#### Towards a science exocortex

Kevin G. Yager*

PAPERS

1958

Self-optimizing Bayesian for continuous flow synthesis process
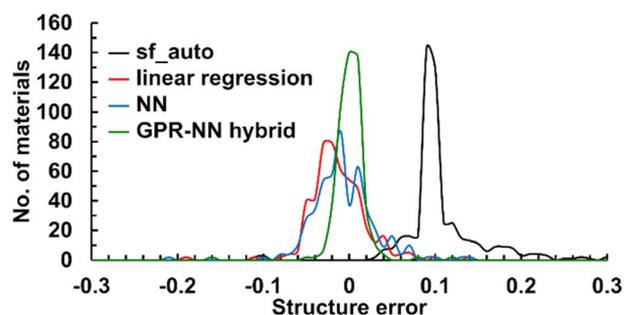
Runzhe Liu, Zihao Wang, Wenbo Yang,* Jinzhe Cao* and Shengyang Tao*

1967

Machine learning the screening factor in the soft bond valence approach for rapid crystal structure estimation
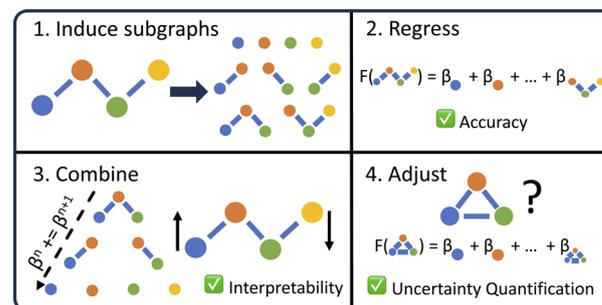
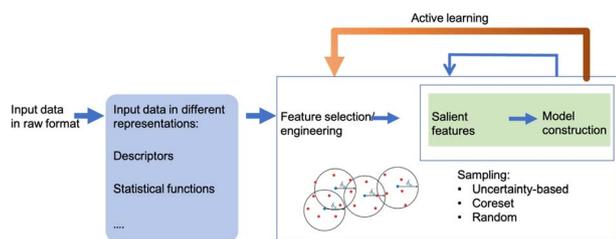Keisuke Kameda,* Takaaki Ariga, Kazuma Ito, Manabu Ihara* and Sergei Manzhos*

1980

Linear graphlet models for accurate and interpretable cheminformatics

Michael Tynes,* Michael G. Taylor, Jan Janssen, Daniel J. Burrill, Danny Perez, Ping Yang* and Nicholas Lubbers*

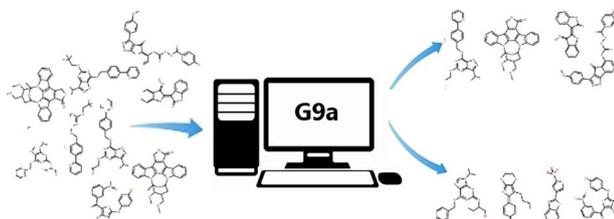## PAPERS

1997

Active learning for regression of structure–property mapping: the importance of sampling and representation

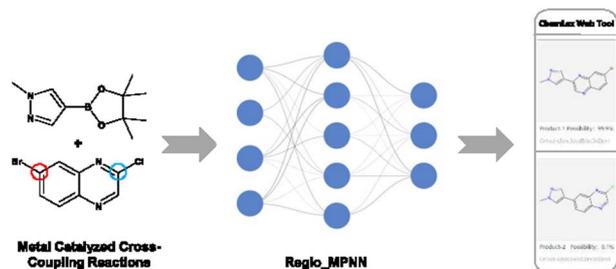Hao Liu,* Berkay Yucel, Baskar Ganapathysubramanian, Surya R. Kalidindi, Daniel Wheeler and Olga Wodo

2010

Application of machine learning for predicting G9a inhibitors

Mariya L. Ivanova,* Nicola Russo, Nadia Djaid and Konstantin Nikolic

2019

Regio-MPNN: predicting regioselectivity for general metal-catalyzed cross-coupling reactions using a chemical knowledge informed message passing neural network

Baochen Li, Yuru Liu, Haibin Sun, Rentao Zhang, Yongli Xie, Klement Foo, Frankie S. Mak, Ruimao Zhang, Tianshu Yu, Sen Lin, Peng Wang and Xiaoxue Wang*

2032

Pellet dispensomixer and pellet distributor: open hardware for nanocomposite space exploration *via* automated material compounding

Miguel Hernández-del-Valle, Jorge Ilarraza-Zuazo, Enrique Dios-Lázaro, Javier Rubio, Joris Audoux and Maciej Haranczyk*

PAPERS

2041

Automated processing of chromatograms: a comprehensive python package with a GUI for intelligent peak identification and deconvolution in chemical reaction analysis

Jan Obořil, Christian P. Haas, Maximilian Lübbesmeyer, Rachel Nicholls, Thorsten Gressling, Klavs F. Jensen,* Giulio Volpin* and Julius Hillenbrand*
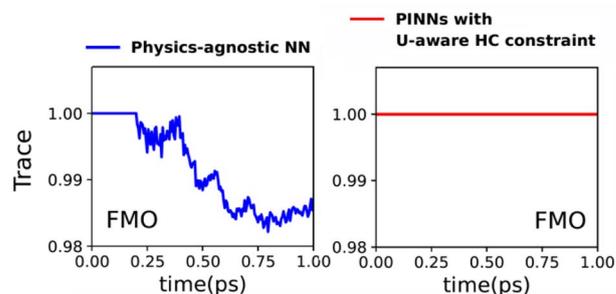

Automated Processing and Analysis of HPLC Chromatograms

✓ open-source ✓ intelligent peak picking
✓ web-based GUI ✓ peak purity check
✓ baseline correction ✓ peak deconvolution

2052

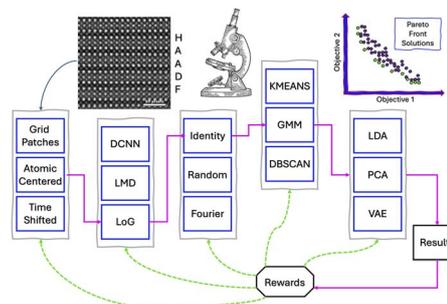**Physics-informed neural networks and beyond: enforcing physical constraints in quantum dissipative dynamics**

Arif Ullah,* Yu Huang, Ming Yang and Pavlo O. Dral*

2061

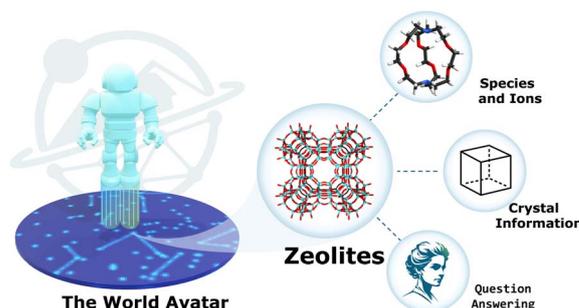**Physics-based reward driven image analysis in microscopy**

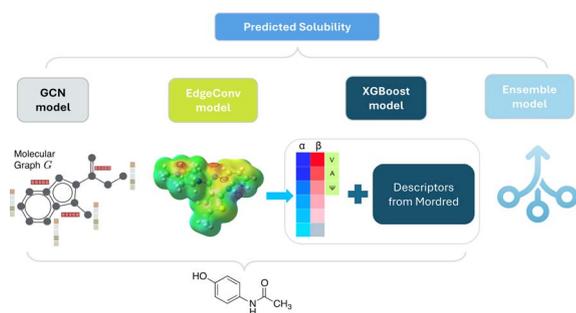K. Barakati,* Hui Yuan, Amit Goyal and S. V. Kalinin*

2070

Knowledge graph representation of zeolitic crystalline materials

Aleksandar Kondinski, Pavlo Rutkevych, Laura Pascazio, Dan N. Tran, Feroz Farazi, Srishti Ganguly and Markus Kraft*

PAPERS

PAPERS

Exploring inhomogeneous surfaces: Ti-rich SrTiO₃(110) reconstructions via active learning

Ralf Wanzenböck, Esther Heid, Michele Riva,
Giada Franceschi, Alexander M. Imre, Jesús Carrete,
Ulrike Diebold and Georg K. H. Madsen*