Open Access Article. Published on 10 July 2025. Downloaded on 12/28/2025 7:26:39 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

Digital Discovery

rsc.li/digitaldiscovery

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

IN THIS ISSUE

ISSN 2635-098X CODEN DDIIAI 4(7) 1653–1976 (2025)

Cover
See Milad Abolhasani *et al.*, pp. 1722–1733. Image reproduced by permission of Milad Abolhasani from *Digital Discovery*, 2025, **4**, 1722.

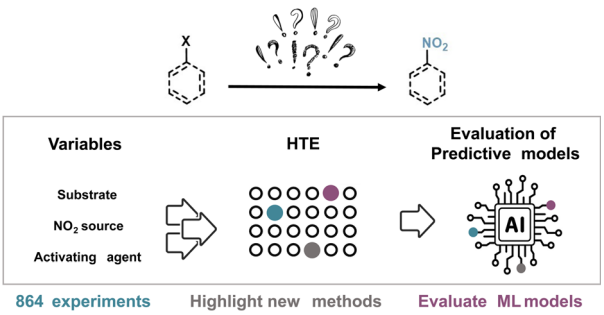
Inside cover
See Kazunori Nishio, Taro Hitosugi *et al.*, pp. 1734–1742. Image reproduced by permission of Taro Hitosugi from *Digital Discovery*, 2025, **4**, 1734.

COMMUNICATION

1662

Investigation of arene and heteroarene nitration supported by high-throughput experimentation and machine learning

Taline Kerackian,* Clément Wespiser, Matthieu Daniel, Eric Pasquinet and Eugénie Romero*

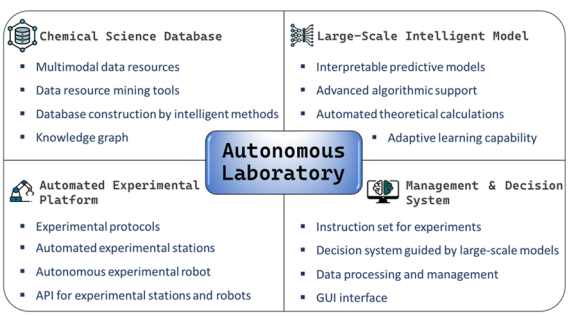


PERSPECTIVE

1672

Autonomous laboratories in China: an embodied intelligence-driven platform to accelerate chemical discovery

Jinpeng Li, Chuxuan Ding, Daobin Liu,* Linjiang Chen and Jun Jiang*



View Article Online

ROYAL SOCIETY OF CHEMISTRY

NEW JOURNAL

RSC Applied Interfaces

GOLD OPEN ACCESS

Interfacial and surface research with an applied focus

Interdisciplinary and open access

rsc.li/RSCApplInter

Fundamental questions
Elemental answers

Registered charity number: 207890

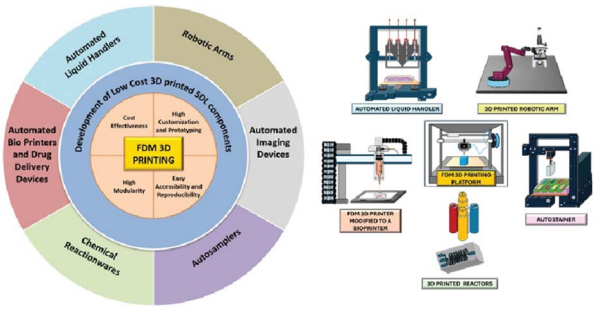
Open Access Article. Published on 10 July 2025. Downloaded on 12/28/2025 7:26:39 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

REVIEW

1685

Democratizing self-driving labs: advances in low-cost 3D printing for laboratory automation

Sayan Doloi, Maloy Das, Yujia Li, Zen Han Cho, Xingchi Xiao, John V. Hanna, Matthew Osvaldo and Leonard Ng Wei Tat*

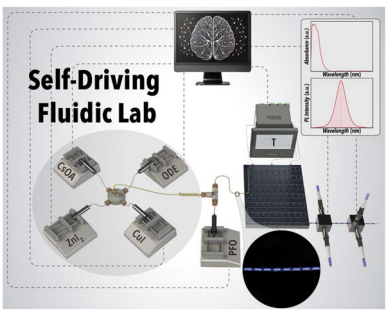


PAPERS

1722

A self-driving fluidic lab for data-driven synthesis of lead-free perovskite nanocrystals

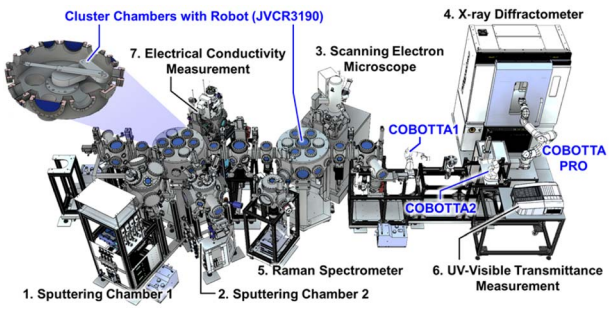
Sina Sadeghi, Karl Mattsson, Joshua Glasheen, Victoria Lee, Christine Stark, Pragyan Jha, Nikolai Mukhin, Junbin Li, Arup Ghorai, Negin Orouji, Christopher H. J. Moran, Alireza Velayati, Jeffrey A. Bennett, Richard B. Canty, Kristofer G. Reyes and Milad Abolhasani*



1734

A digital laboratory with a modular measurement system and standardized data format

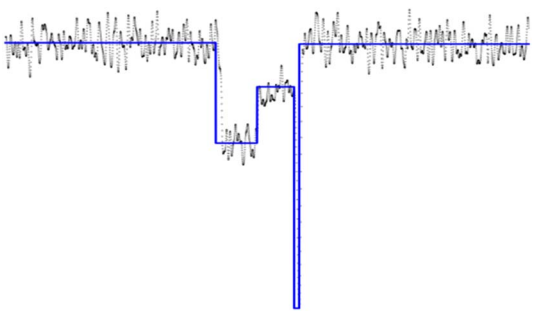
Kazunori Nishio,* Akira Aiba, Kei Takihara, Yota Suzuki, Ryo Nakayama, Shigeru Kobayashi, Akira Abe, Haruki Baba, Shinichi Katagiri, Kazuki Omoto, Kazuki Ito, Ryota Shimizu and Taro Hitosugi*



1743

Nano Trees: nanopore signal processing and sublevel fitting using decision trees

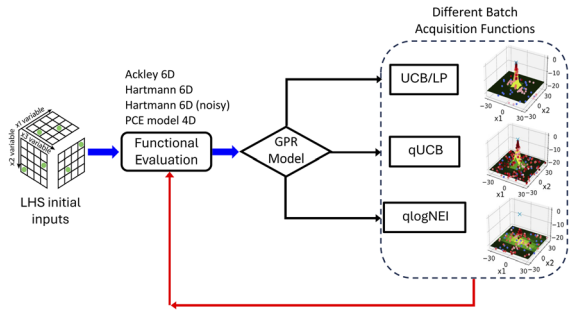
Deekshant Wadhwa, Philipp Mensing, James Harden, Paula Branco, Vincent Tabard-Cossa and Kyle Briggs*



Open Access Article. Published on 10 July 2025. Downloaded on 12/28/2025 7:26:39 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

PAPERS

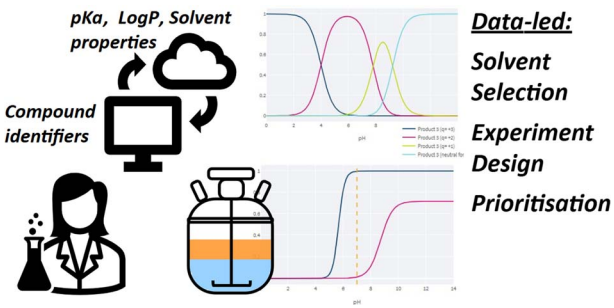
1751



Choosing a suitable acquisition function for batch Bayesian optimization: comparison of serial and Monte Carlo approaches

Imon Mia, Mark Lee, Weijie Xu, William Vandenberghe and Julia W. P. Hsu*

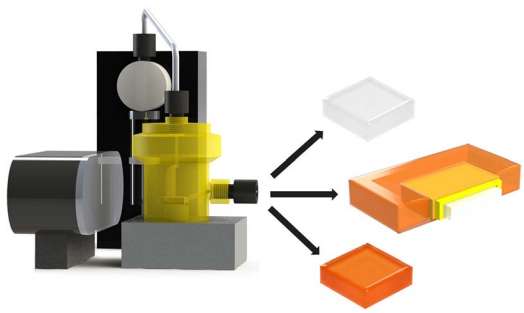
1763



A digital tool for liquid–liquid extraction process design

George Karageorgis,* Simone Tomasi, Elliot H. E. Farrar, Maxime Tarrago and Tabassum Malik

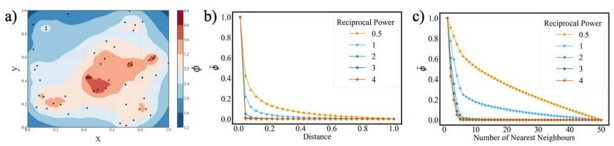
1772



Digital flow platform for the synthesis of high-quality multi-material perovskites

Diego Iglesias, Cristopher Tinajero, Simone Marchetti, Jaume Luis-Gómez, Raúl Martinez-Cuenca, Jose F. Fuentes-Ballesteros, Clara A. Aranda, Alejandro Martínez Serra, María C. Asensio, Rafael Abargues, Pablo P. Boix, Marcileia Zanatta and Victor Sans*

1784



Computation-guided exploration of the reaction parameter space of *N*,*N*-dimethylformamide hydrolysis

Ignas Pakamorė* and Ross S. Forgan

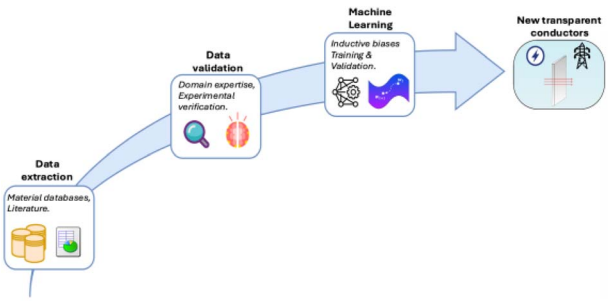
This journal is © The Royal Society of Chemistry 2025

Open Access Article. Published on 10 July 2025. Downloaded on 12/28/2025 7:26:39 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

1794

Assessing data-driven predictions of band gap and electrical conductivity for transparent conducting materials

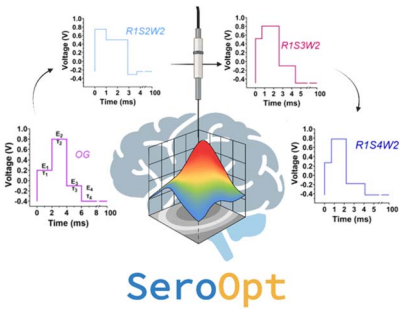
Federico Ottomano, John Y. Goulermas, Vladimir Gusev, Rahul Savani,* Michael W. Gaultois, Troy D. Manning, Hai Lin, Teresa Partida Manzanera, Emmeline G. Poole, Matthew S. Dyer, John B. Claridge, Jon Alaria, Luke M. Daniels, Su Varma, David Rimmer, Kevin Sanderson and Matthew J. Rosseinsky*



1812

Machine-learning-guided design of electroanalytical pulse waveforms

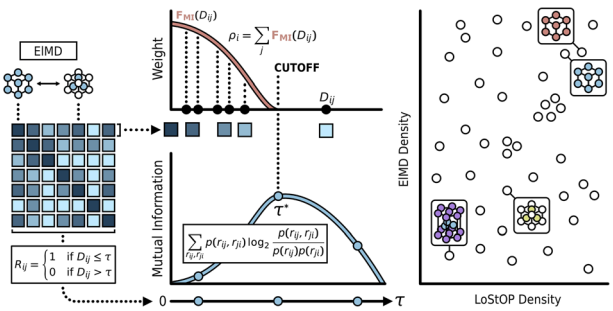
Cameron S. Movassaghi,* Katie A. Perrotta, Maya E. Curry, Audrey N. Nashner, Katherine K. Nguyen, Mila E. Wesely, Miguel Alcañiz Fillol, Chong Liu, Aaron S. Meyer and Anne M. Andrews*



1833

Mutual information informed novelty estimation of materials along chemical and structural axes

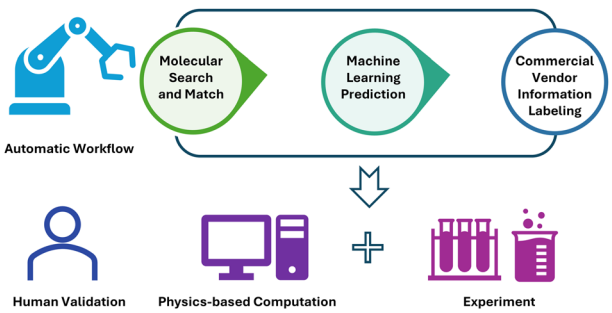
Andrew R. Falkowski* and Taylor D. Sparks



1844

RedCat, an automated discovery workflow for aqueous organic electrolytes

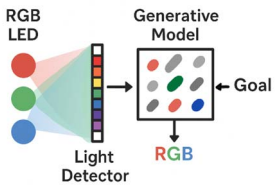
Murat Cihan Sorkun, Xuan Zhou, Joannes Murigneux, Nicola Menegazzo, Ayush Kumar Narsaria, David Thanoon, Peter A. A. Klusener, Kaustubh Kaluskar, Sharan Shetty, Efstathios Barmpoutsis and Süleyman Er*



Open Access Article. Published on 10 July 2025. Downloaded on 12/28/2025 7:26:39 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

PAPERS

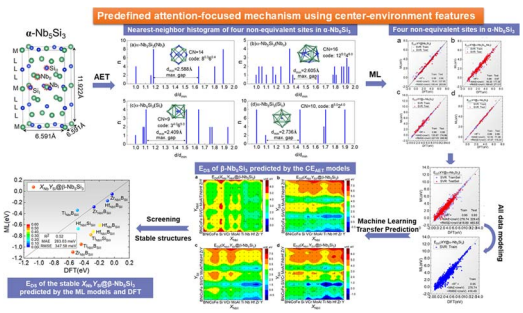
1856



Solving an inverse problem with generative models

John R. Kitchin*

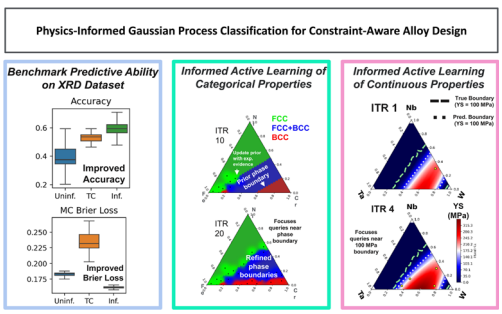
1870



Predefined attention-focused mechanism using center-environment features: a machine learning study of alloying effects on the stability of Nb_5Si_3 alloys

Yuchao Tang, Bin Xiao, Shuizhou Chen, Quan Qian and Yi Liu*

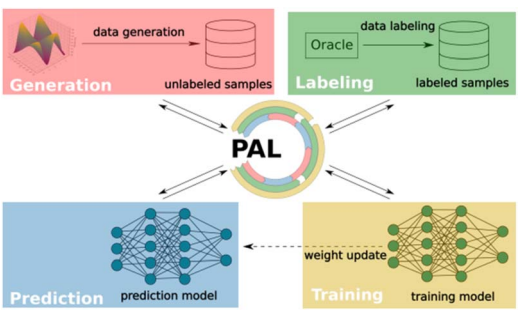
1884



Physics-informed Gaussian process classification for constraint-aware alloy design

Christofer Hardcastle, Ryan O'Mullan, Raymundo Arróyave and Brent Vela*

1901



PAL – parallel active learning for machine-learned potentials

Chen Zhou, Marlen Neubert, Yuri Koide, Yumeng Zhang, Van-Quan Vuong, Tobias Schlöder, Stefanie Dehnen and Pascal Friederich*

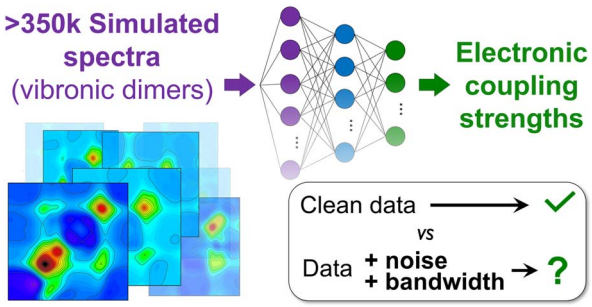
This journal is © The Royal Society of Chemistry 2025

Open Access Article. Published on 10 July 2025. Downloaded on 12/28/2025 7:26:39 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

1912

Using machine learning to map simulated noisy and laser-limited multidimensional spectra to molecular electronic couplings

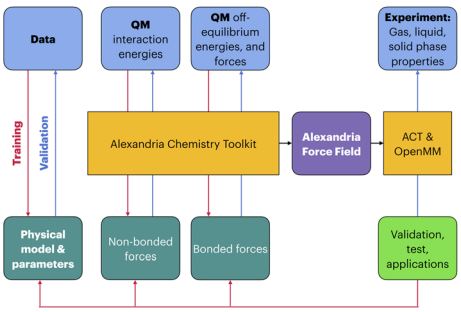
Jonathan D. Schultz,* Kelsey A. Parker,* Bashir Sbaiti and David N. Beratan



1925

Evolutionary machine learning of physics-based force fields in high-dimensional parameter-space

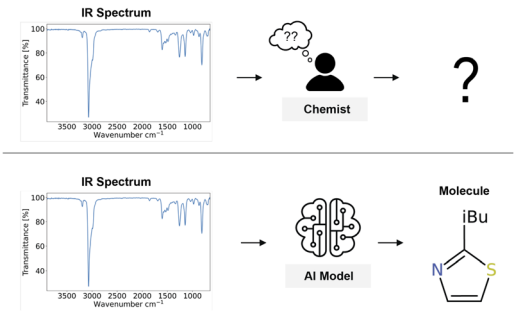
David van der Spoel,* Julián Marrades, Kristian Kříž, A. Najla Hosseini, Alfred T. Nordman, João Paulo, Marie-Madeleine Walz, Paul J. van Maaren and Mohammad M. Ghahremanpour*



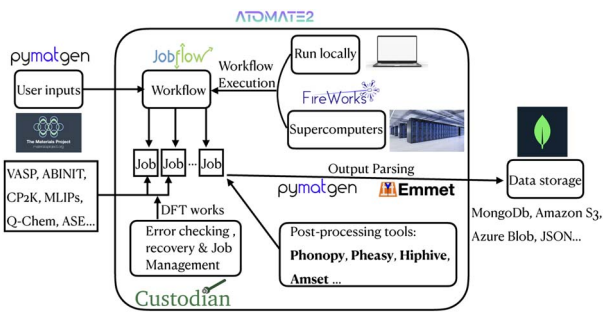
1936

Setting new benchmarks in AI-driven infrared structure elucidation

Marvin Alberts,* Federico Zipoli and Teodoro Laino



1944

Atomate2: modular workflows for materials science

A. M. Ganose,* H. Sahasrabuddhe, M. Asta, K. Beck, T. Biswas, A. Bonkowski, J. Bustamante, X. Chen, Y. Chiang, D. C. Chrzan, J. Clary, O. A. Cohen, C. Ertural, M. C. Gallant, J. George, S. Gerits, R. E. A. Goodall, R. D. Guha, G. Hautier, M. Horton, T. J. Inizan, A. D. Kaplan, R. S. Kingsbury, M. C. Kuner, B. Li, X. Linn, M. J. McDermott, R. S. Mohanakrishnan, A. N. Naik, J. B. Neaton, S. M. Parmar, K. A. Persson, G. Petretto, T. A. R. Purcell, F. Ricci, B. Rich, J. Riebesell, G.-M. Rignanese, A. S. Rosen, M. Scheffler, J. Schmidt, J.-X. Shen, A. Sobolev, R. Sundararaman, C. Tezak, V. Trinquet, J. B. Varley, D. Vigil-Fowler, D. Wang, D. Waroquiers, M. Wen, H. Yang, H. Zheng, J. Zheng, Z. Zhu and A. Jain*