

# Digital Discovery

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## IN THIS ISSUE

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



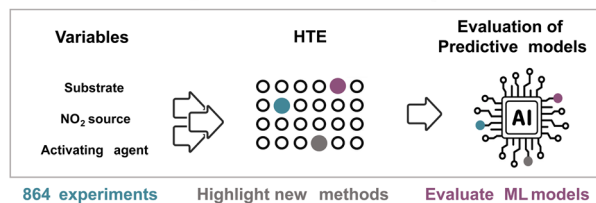
**Inside cover**  
See Kazunori Nishio, Taro Hitosugi *et al.*, pp. 1734–1742. Image reproduced by permission of Taro Hitosugi from *Digital Discovery*, 2025, 4, 1734.

## 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\*

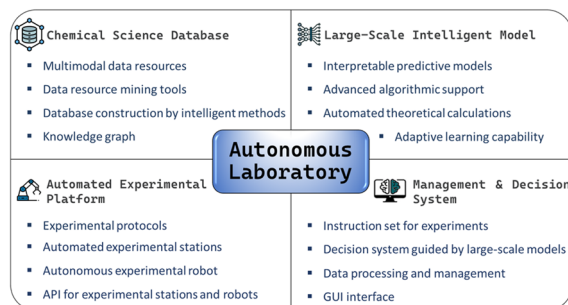


## PERSPECTIVE

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\*



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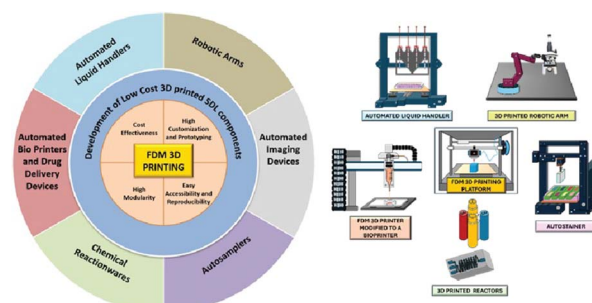
Fundamental questions  
Elemental answers

## 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\*

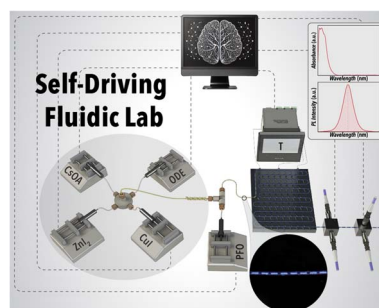


## PAPERS

1722

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

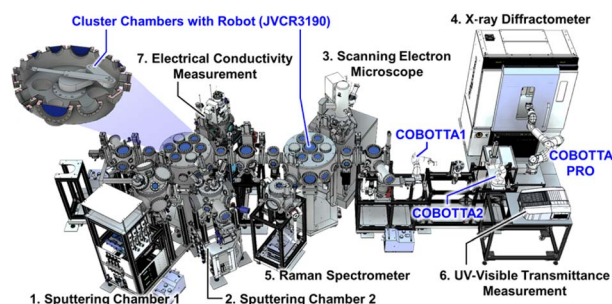
Sina Sadeghi, Karl Mattsson, Joshua Glasheen, Victoria Lee, Christine Stark, Pragyan Jha, Nikolai Mukhin, Junbin Li, Arup Ghorai, Negin Orouji, Christopher H. J. Moran, Alireza Velayati, Jeffrey A. Bennett, Richard B. Canty, Kristofer G. Reyes and Milad Abolhasani\*



1734

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

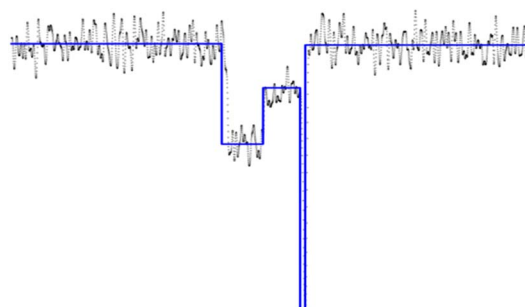
Kazunori Nishio,\* Akira Aiba, Kei Takihara, Yota Suzuki, Ryo Nakayama, Shigeru Kobayashi, Akira Abe, Haruki Baba, Shinichi Katagiri, Kazuki Omoto, Kazuki Ito, Ryota Shimizu and Taro Hitosugi\*



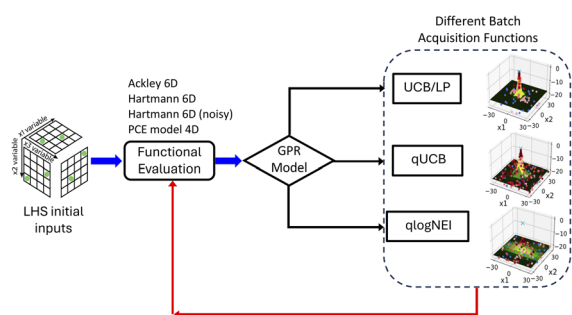
1743

## 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\*



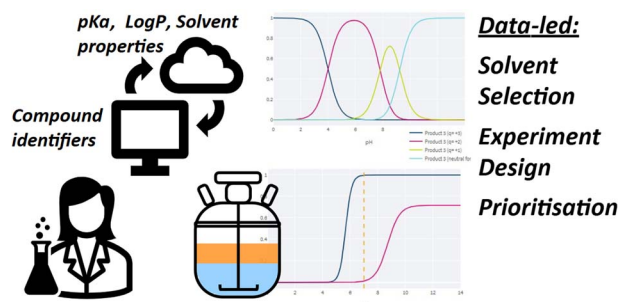
1751



## 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\*

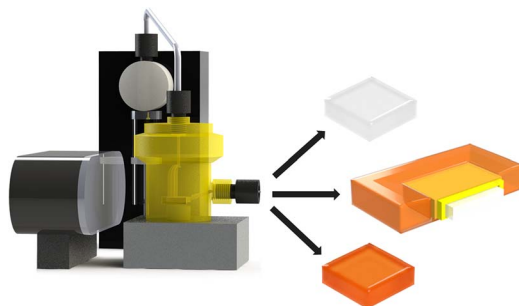
1763



## A digital tool for liquid–liquid extraction process design

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

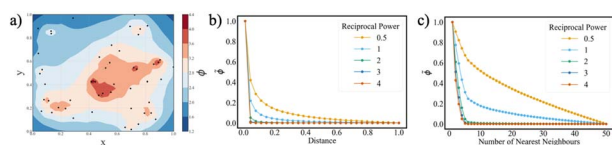
1772



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

Diego Iglesias, Christopher Tinajero, Simone Marchetti, Jaime Luis-Gómez, Raúl Martínez-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

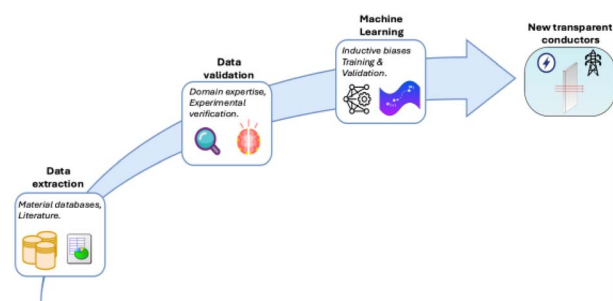
Ignas Pakamoré\* and Ross S. Forgan



1794

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

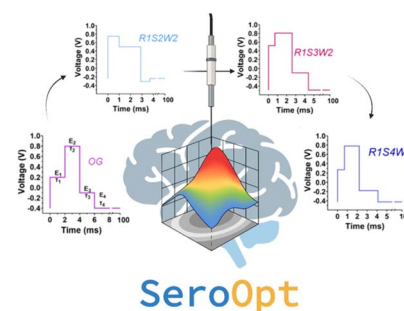
Federico Ottomano, John Y. Goulermas, Vladimir Gusev, Rahul Savani,\* Michael W. Gaultois, Troy D. Manning, Hai Lin, Teresa Partida Manzanera, Emmeline G. Poole, Matthew S. Dyer, John B. Claridge, Jon Alaria, Luke M. Daniels, Su Varma, David Rimmer, Kevin Sanderson and Matthew J. Rosseinsky\*



1812

## Machine-learning-guided design of electroanalytical pulse waveforms

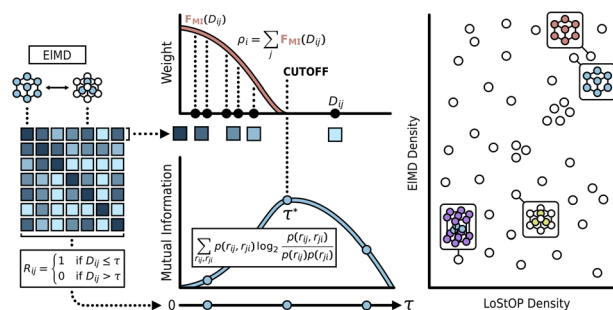
Cameron S. Movassaghi,\* Katie A. Perrotta, Maya E. Curry, Audrey N. Nashner, Katherine K. Nguyen, Mila E. Wesely, Miguel Alcañiz Fillol, Chong Liu, Aaron S. Meyer and Anne M. Andrews\*



1833

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

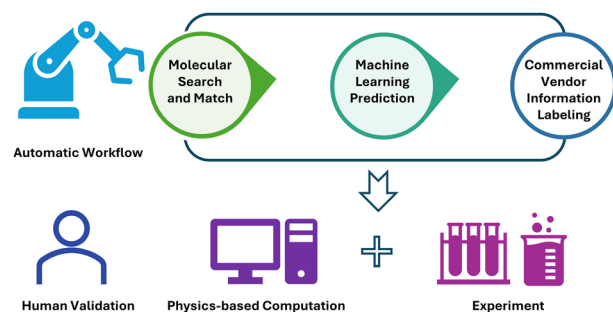
Andrew R. Falkowski\* and Taylor D. Sparks



1844

## RedCat, an automated discovery workflow for aqueous organic electrolytes

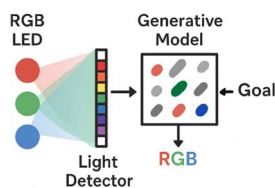
Murat Cihan Sorkun, Xuan Zhou, Joannes Murigneux, Nicola Menegazzo, Ayush Kumar Narsaria, David Thanoon, Peter A. A. Klusener, Kaustubh Kaluskar, Sharan Shetty, Efsthios Barmopoulos and Süleyman Er\*



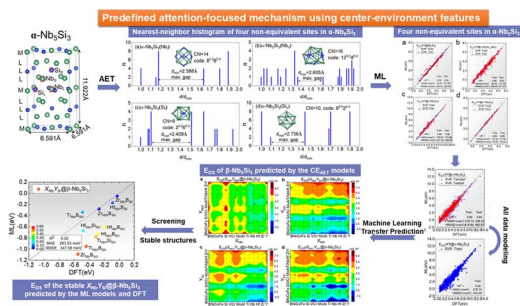
1856

## Solving an inverse problem with generative models

John R. Kitchin\*

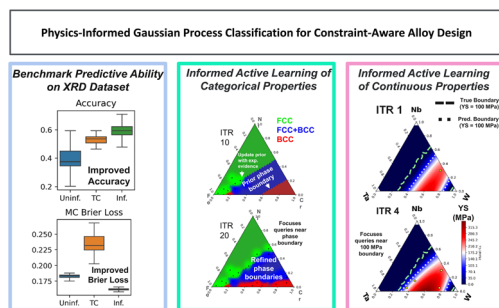


1870

Predefined attention-focused mechanism using center-environment features: a machine learning study of alloying effects on the stability of Nb<sub>5</sub>Si<sub>3</sub> alloys

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

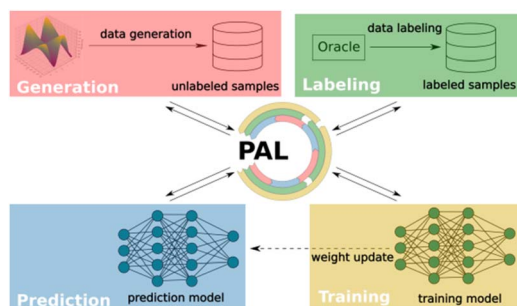
1884



## 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

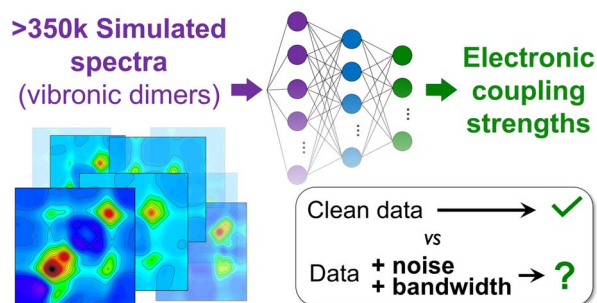
Chen Zhou, Marlen Neubert, Yuri Koide, Yumeng Zhang, Van-Quan Vuong, Tobias Schlöder, Stefanie Dehnen and Pascal Friederich\*



1912

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

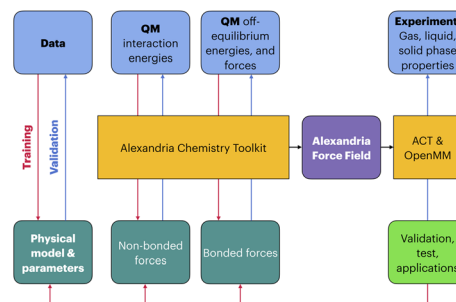
Jonathan D. Schultz,\* Kelsey A. Parker,\* Bashir Sbaiti and David N. Beratan



1925

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

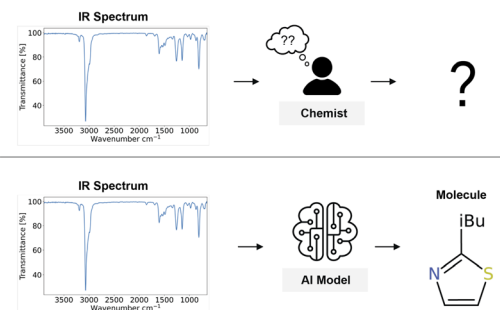
David van der Spoel,\* Julián Marrades, Kristian Kříž, A. Najla Hosseini, Alfred T. Nordman, João Paulo, Marie-Madeleine Walz, Paul J. van Maaren and Mohammad M. Ghahremanpour\*



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\*

