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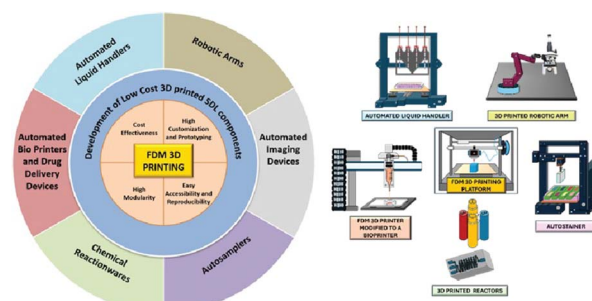
Fundamental questions
Elemental answers

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*

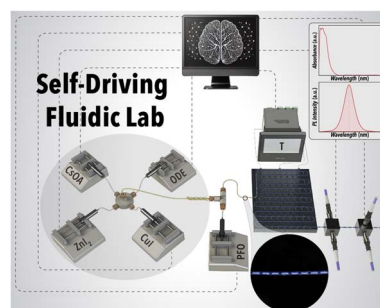


PAPERS

1722

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

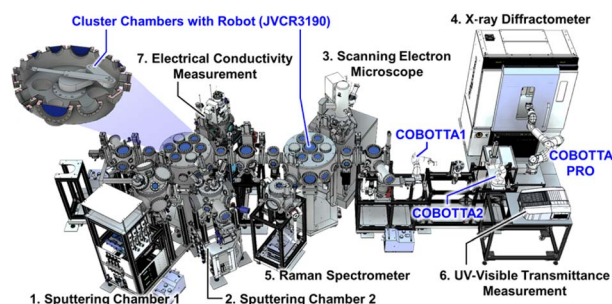
Sina Sadeghi, Karl Mattsson, Joshua Glasheen, Victoria Lee, Christine Stark, Pragyan Jha, Nikolai Mukhin, Junbin Li, Arup Ghorai, Negin Orouji, Christopher H. J. Moran, Alireza Velayati, Jeffrey A. Bennett, Richard B. Canty, Kristofer G. Reyes and Milad Abolhasani*



1734

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

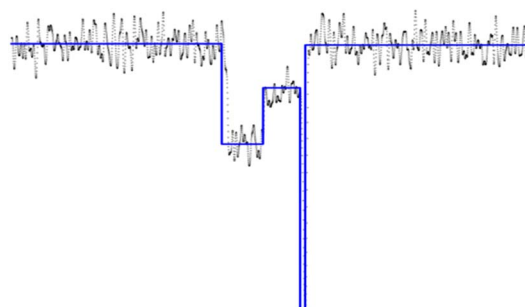
Kazunori Nishio,* Akira Aiba, Kei Takihara, Yota Suzuki, Ryo Nakayama, Shigeru Kobayashi, Akira Abe, Haruki Baba, Shinichi Katagiri, Kazuki Omoto, Kazuki Ito, Ryota Shimizu and Taro Hitosugi*



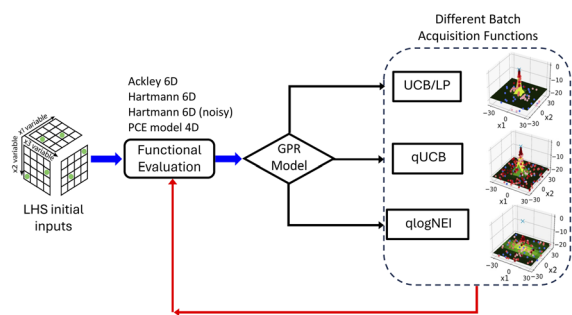
1743

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*



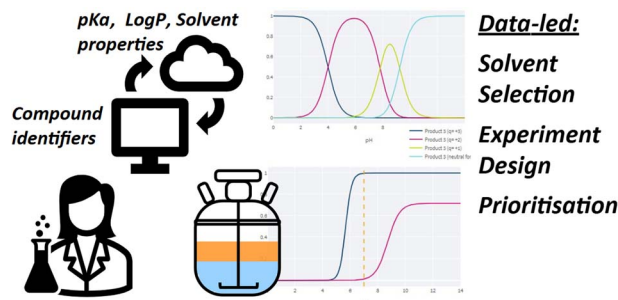
1751



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*

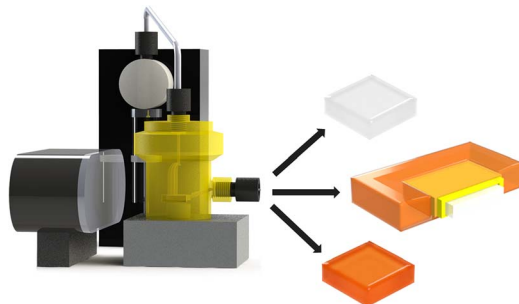
1763



A digital tool for liquid–liquid extraction process design

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

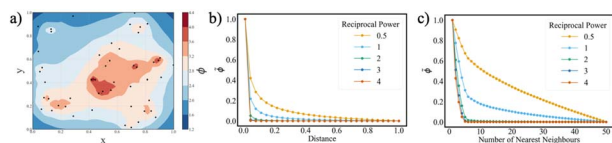
1772



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

Diego Iglesias, Christopher Tinajero, Simone Marchetti, Jaume 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

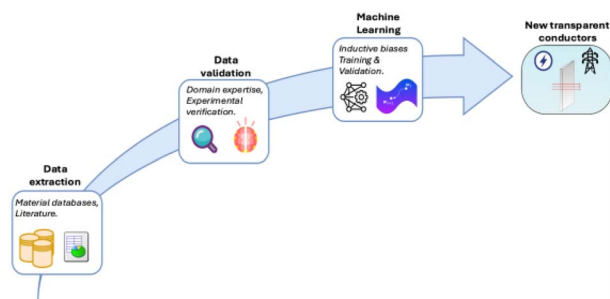
Ignas Pakamoré* and Ross S. Forgan



1794

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

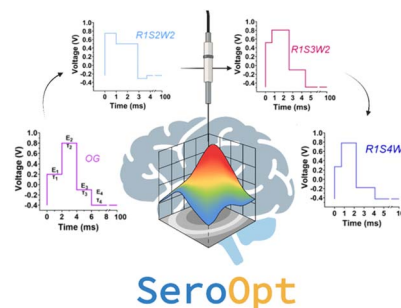
Federico Ottomano, John Y. Goulermas, Vladimir Gusev, Rahul Savani,* Michael W. Gaultois, Troy D. Manning, Hai Lin, Teresa Partida Manzanera, Emmeline G. Poole, Matthew S. Dyer, John B. Claridge, Jon Alaria, Luke M. Daniels, Su Varma, David Rimmer, Kevin Sanderson and Matthew J. Rosseinsky*



1812

Machine-learning-guided design of electroanalytical pulse waveforms

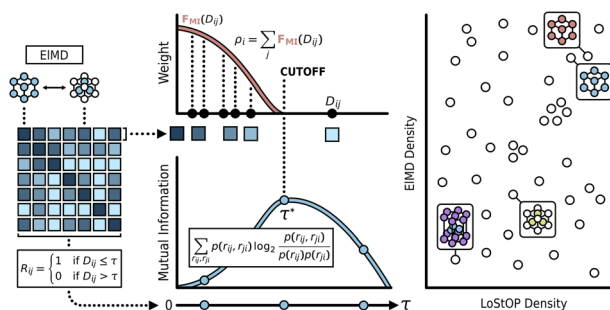
Cameron S. Movassaghi,* Katie A. Perrotta, Maya E. Curry, Audrey N. Nashner, Katherine K. Nguyen, Mila E. Wesely, Miguel Alcañiz Fillol, Chong Liu, Aaron S. Meyer and Anne M. Andrews*



1833

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

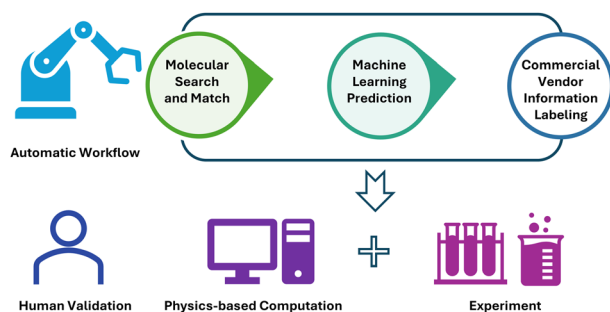
Andrew R. Falkowski* and Taylor D. Sparks



1844

RedCat, an automated discovery workflow for aqueous organic electrolytes

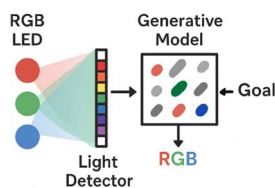
Murat Cihan Sorkun, Xuan Zhou, Joannes Murigneux, Nicola Menegazzo, Ayush Kumar Narsaria, David Thanoon, Peter A. A. Klusener, Kaustubh Kaluskar, Sharan Shetty, Efsthios Barmopoulos and Süleyman Er*



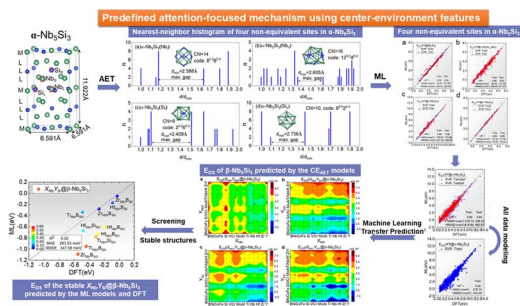
1856

Solving an inverse problem with generative models

John R. Kitchin*

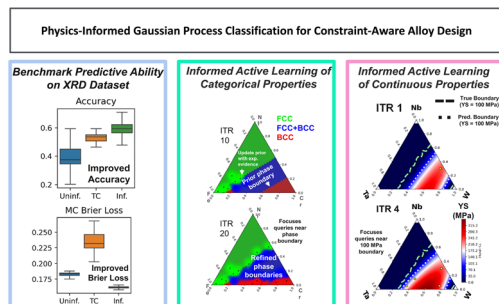


1870

Predefined attention-focused mechanism using center-environment features: a machine learning study of alloying effects on the stability of Nb₅Si₃ alloys

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

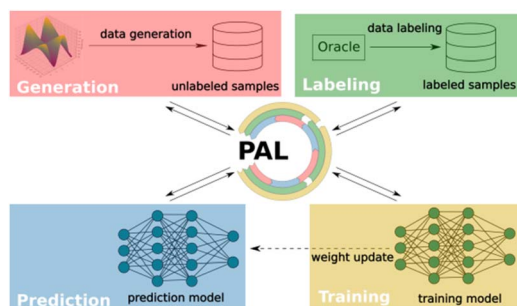
1884



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

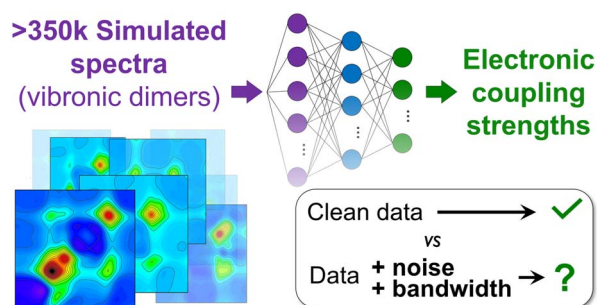
Chen Zhou, Marlen Neubert, Yuri Koide, Yumeng Zhang, Van-Quan Vuong, Tobias Schlöder, Stefanie Dehnen and Pascal Friederich*



1912

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

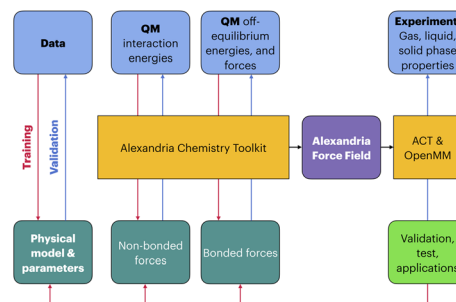
Jonathan D. Schultz,* Kelsey A. Parker,* Bashir Sbaiti and David N. Beratan



1925

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

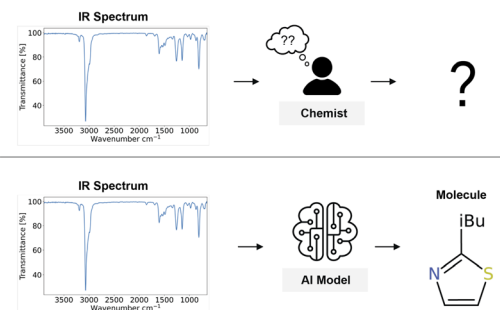
David van der Spoel,* Julián Marrades, Kristian Kříž, A. Najla Hosseini, Alfred T. Nordman, João Paulo, Marie-Madeleine Walz, Paul J. van Maaren and Mohammad M. Ghahremanpour*



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*

