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IN THIS ISSUE

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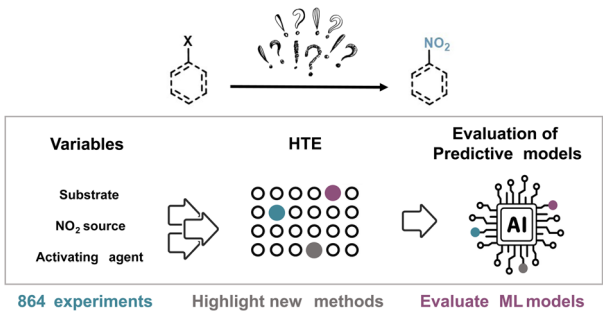
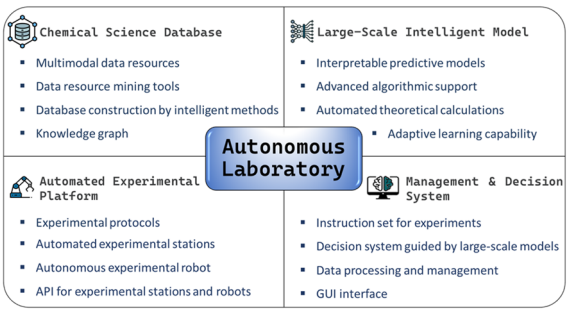
Cover
See Milad Abolhasani *et al.*, pp. 1722–1733. Image reproduced by permission of Milad Abolhasani from *Digital Discovery*, 2025, **4**, 1722.

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



PERSPECTIVE



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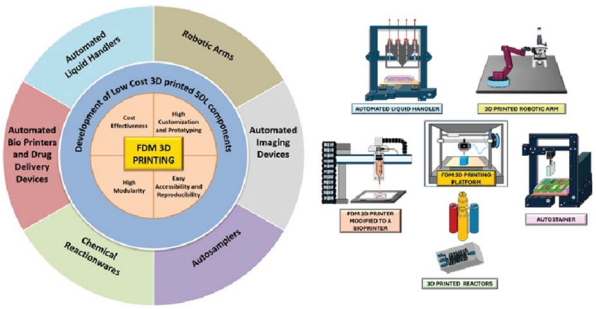
REVIEW



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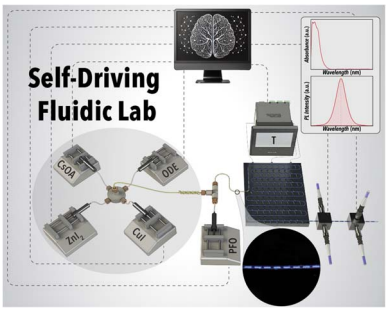

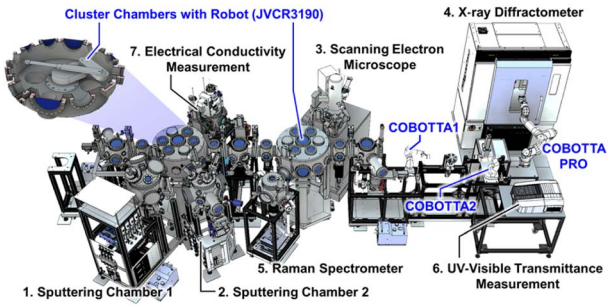

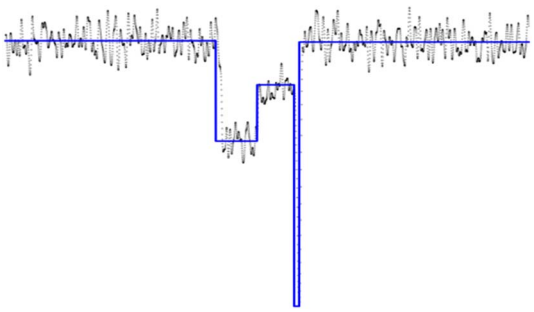

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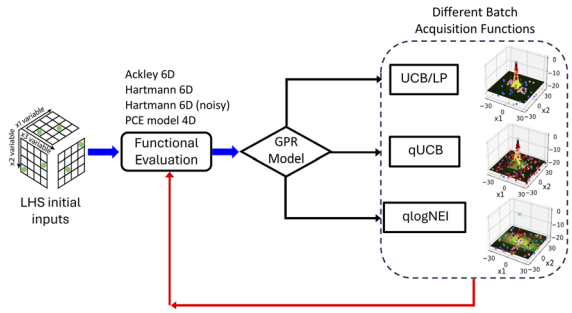
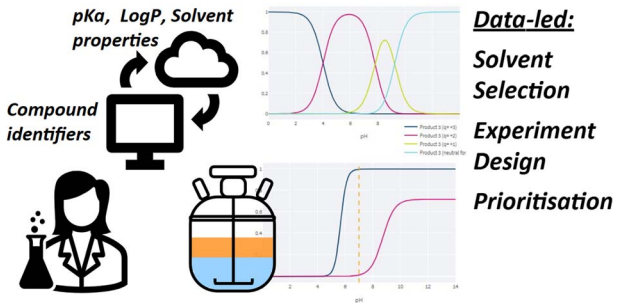
1751



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*

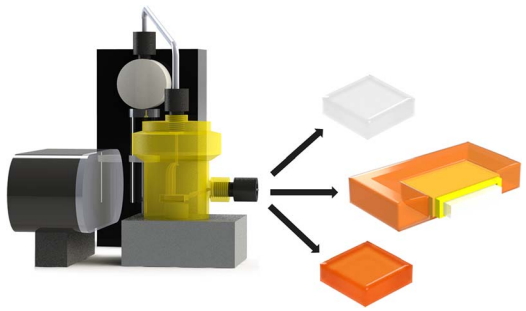
1763



A digital tool for liquid–liquid extraction process design

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

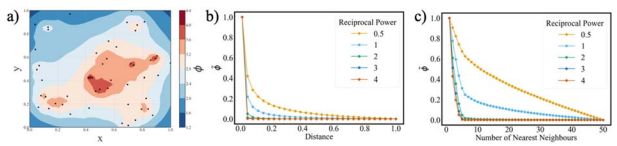
1772



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

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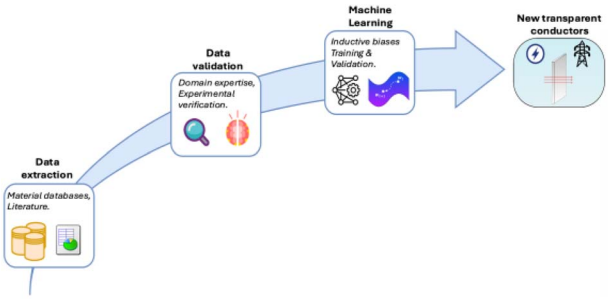

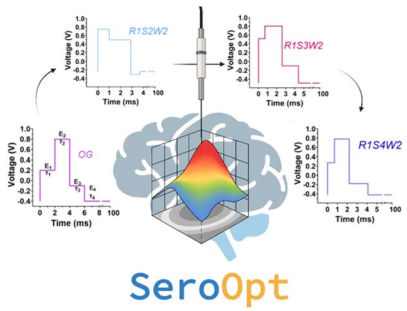

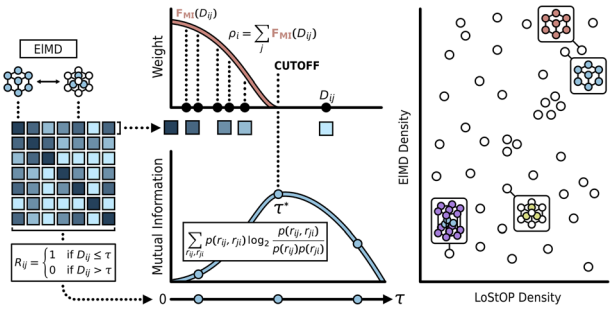

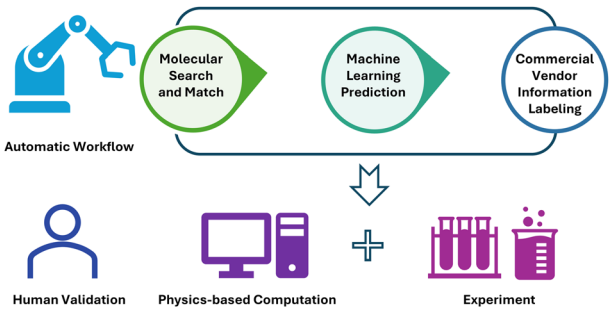

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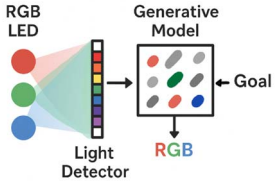
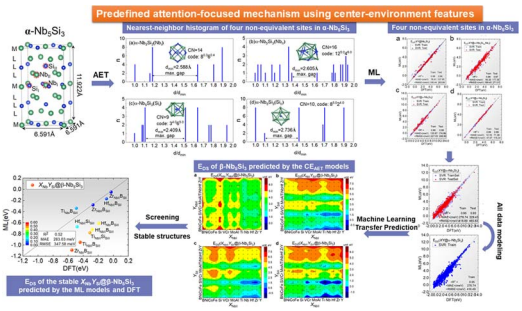
1856



Solving an inverse problem with generative models

John R. Kitchin*

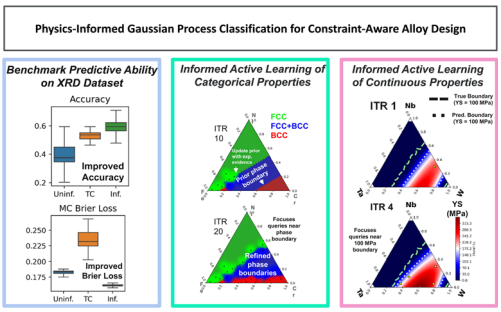
1870



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*

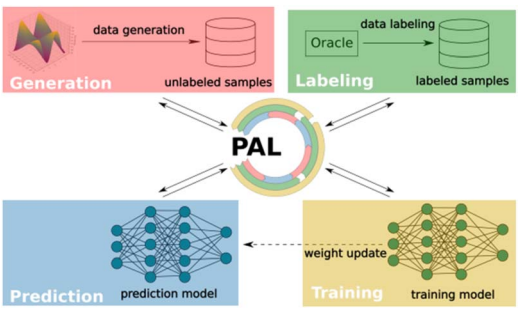
1884



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*

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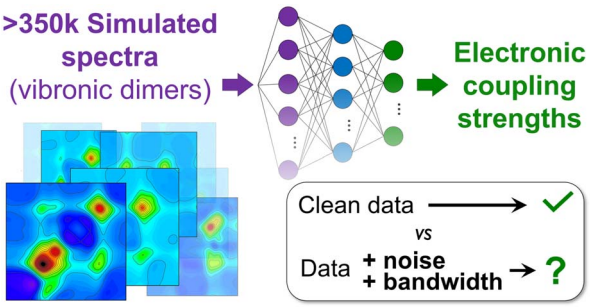
1912

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

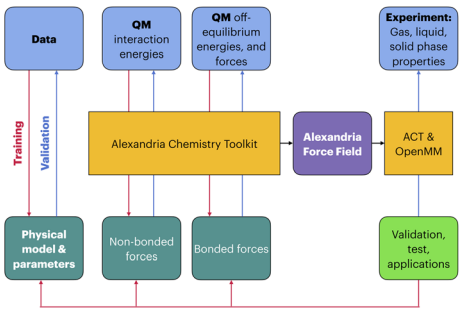
Jonathan D. Schultz,* Kelsey A. Parker,* Bashir Sbaiti and David N. Beratan



1925

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

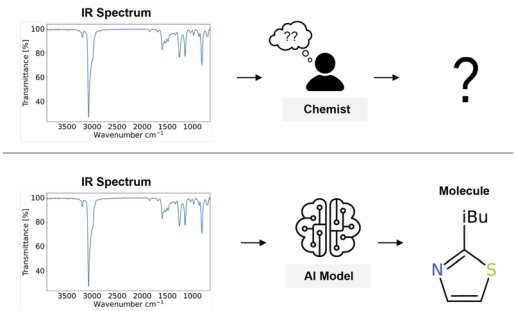
David van der Spoel,* Julián Marrades, Kristian Kříž, A. Najla Hosseini, Alfred T. Nordman, João Paulo, Marie-Madeleine Walz, Paul J. van Maaren and Mohammad M. Ghahremanpour*



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*