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IN THIS ISSUE

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Cover
See Matthew D. Witman and Peter Schindler, pp. 625–635. Image reproduced by permission of David Witman and Peter Schindler from *Digital Discovery*, 2025, **4**, 625.

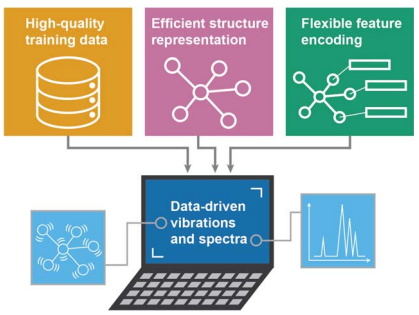
Inside cover
See Linjiang Chen, Fei Zhang, Weiwei Shang, Jun Jiang *et al.*, pp. 636–652. Image reproduced by permission of Jun Jiang from *Digital Discovery*, 2025, **4**, 636.

REVIEW

584

AI-powered exploration of molecular vibrations, phonons, and spectroscopy

Bowen Han, Ryotaro Okabe, Abhijatmedhi Chotrattanapituk, Mouyang Cheng, Mingda Li* and Yongqiang Cheng*

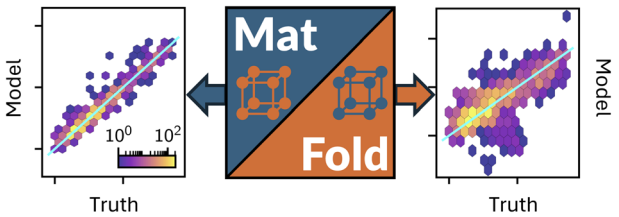


PAPERS

625

MatFold: systematic insights into materials discovery models' performance through standardized cross-validation protocols

Matthew D. Witman* and Peter Schindler*



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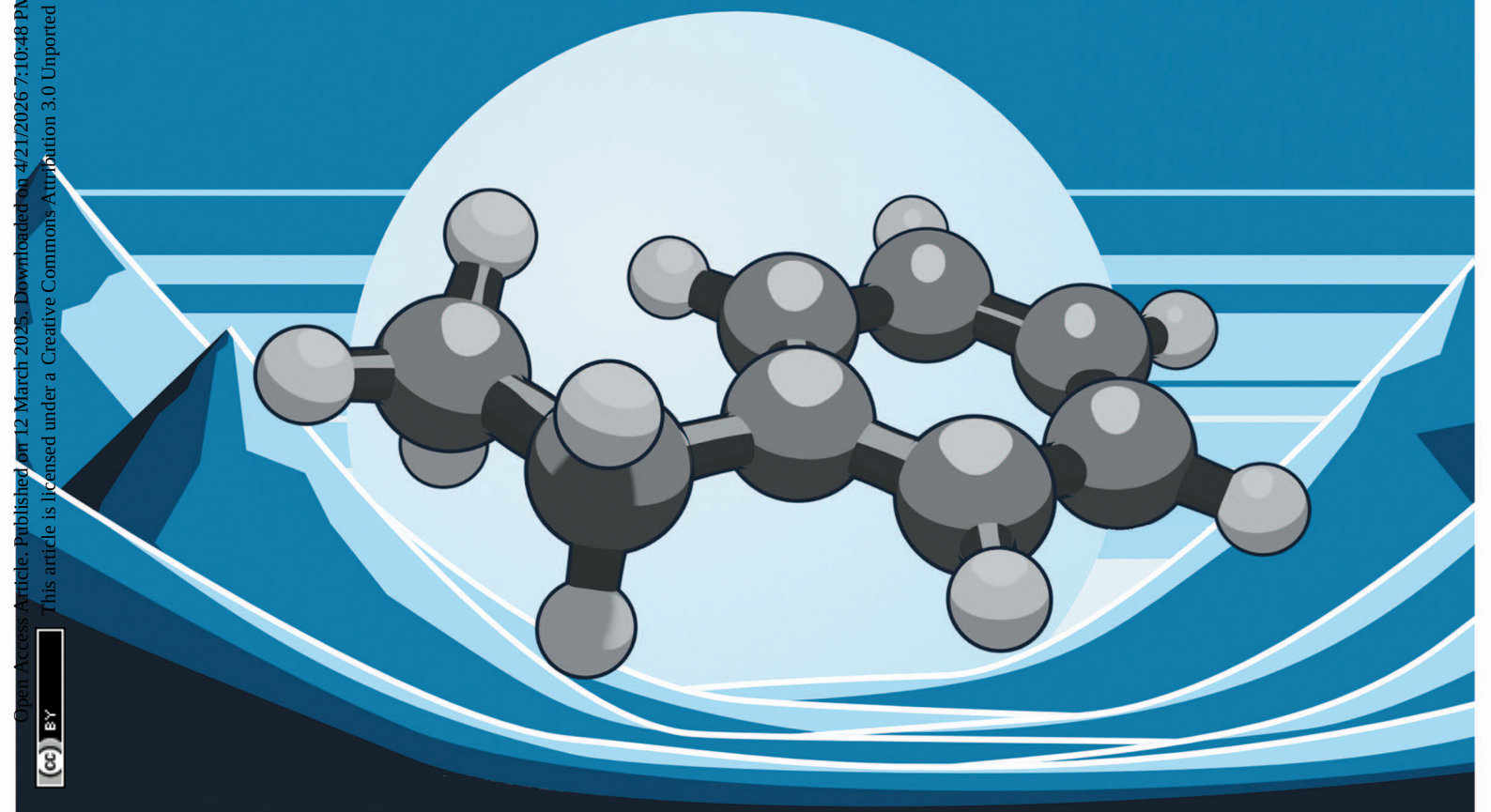
Cheminformatics, Automation and Machine Learning in Chemistry (CAMLC micro-credential)



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PAPERS

636

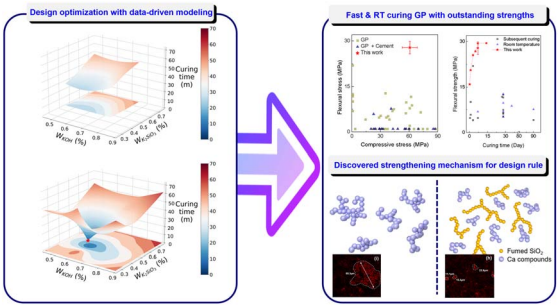
A multi-robot–multi-task scheduling system for autonomous chemistry laboratories

Junyi Zhou, Man Luo, Linjiang Chen,* Qing Zhu, Shan Jiang, Fei Zhang,* Weiwei Shang* and Jun Jiang*

653

Accentuating the ambient curing behavior of geopolymers: metamodel-guided optimization for fast-curing geopolymers with high flexural strength

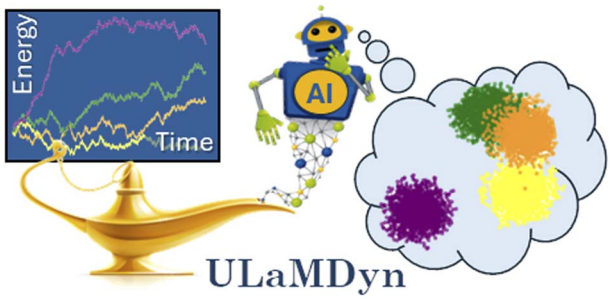
Kyungwon Kim, Hyejeong Song, Sanghun Lee, Hyeongkyu Cho, Hyung Mi Lim and Hyunseok Ko*



666

ULaMDyn: enhancing excited-state dynamics analysis through streamlined unsupervised learning

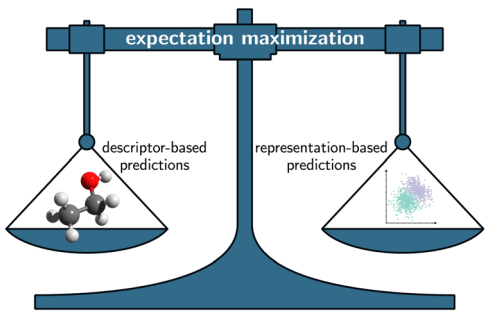
Max Pinheiro Jr,* Matheus de Oliveira Bispo, Rafael S. Mattos, Mariana Telles do Casal, Bidhan Chandra Garain,* Josene M. Toldo, Saikat Mukherjee and Mario Barbatti*



683

Balancing molecular information and empirical data in the prediction of physico-chemical properties

Johannes Zenn,* Dominik Gond, Fabian Jirasek and Robert Bamler



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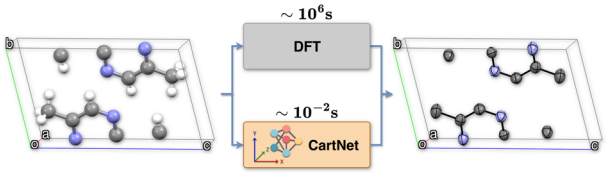
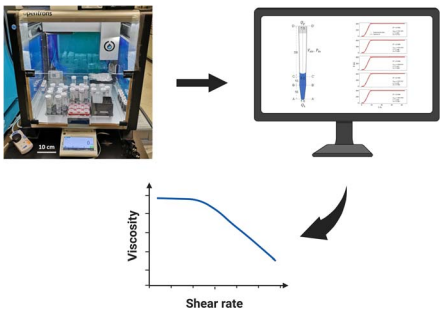
694



A Cartesian encoding graph neural network for crystal structure property prediction: application to thermal ellipsoid estimation

Àlex Solé, Albert Mosella-Montoro, Joan Cardona, Silvia Gómez-Coca,* Daniel Aravena,* Eliseo Ruiz* and Javier Ruiz-Hidalgo*

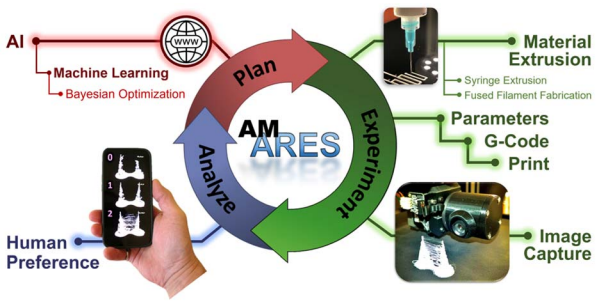
711



Opentrons for automated and high-throughput viscometry

Beatrice W. Soh,* Aniket Chitre, Shu Zheng Tan, Yuhan Wang, Yinqi Yi, Wendy Soh, Kedar Hippalgaonkar and D. Ian Wilson

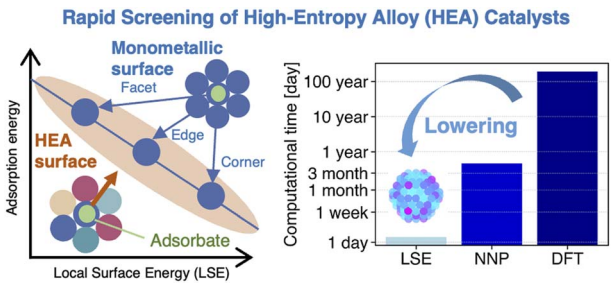
723



Preferential Bayesian optimization improves the efficiency of printing objects with subjective qualities

James R. Deneault, Woojae Kim, Jiseob Kim, Yuzhe Gu, Jorge Chang, Benji Maruyama, Jay I. Myung and Mark A. Pitt*

738



Lowering the exponential wall: accelerating high-entropy alloy catalysts screening using local surface energy descriptors from neural network potentials

Tomoya Shiota,* Kenji Ishihara and Wataru Mizukami*

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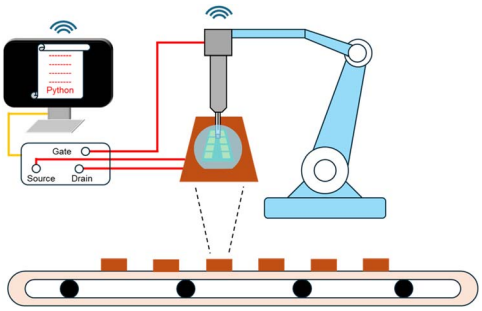
752

An automated electrolyte-gate field-effect transistor test system for rapid screening of multiple sensors

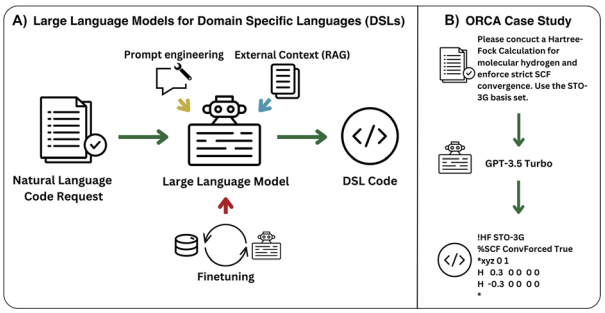
Zhengru Liu, Long Bian, Wenting Shao, Sean I. Hwang and Alexander Star*



762

Developing large language models for quantum chemistry simulation input generation

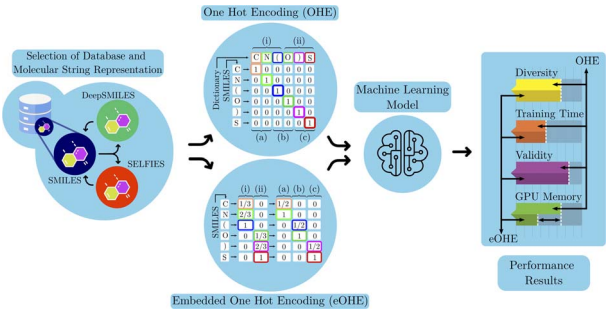
Pieter Floris Jacobs and Robert Pollice*



776

Embedded machine-readable molecular representation for resource-efficient deep learning applications

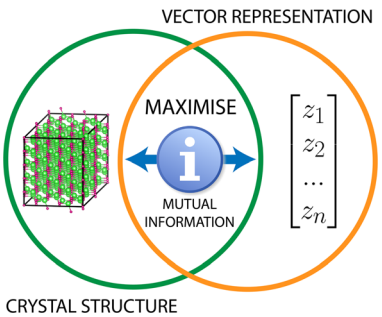
Emilio Nuñez-Andrade,* Isaac Vidal-Daza, James W. Ryan, Rafael Gómez-Bombarelli and Francisco J. Martin-Martinez*



790

Establishing Deep InfoMax as an effective self-supervised learning methodology in materials informatics

Michael Moran, Michael W. Gaultois, Vladimir V. Gusev,* Dmytro Antypov and Matthew J. Rosseinsky*



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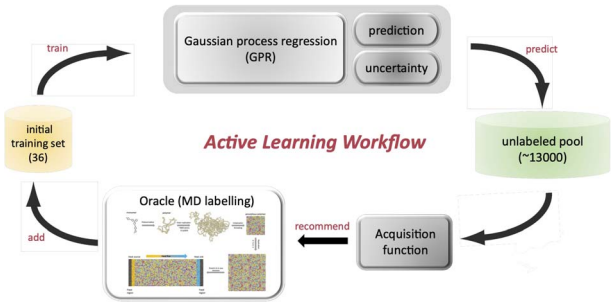
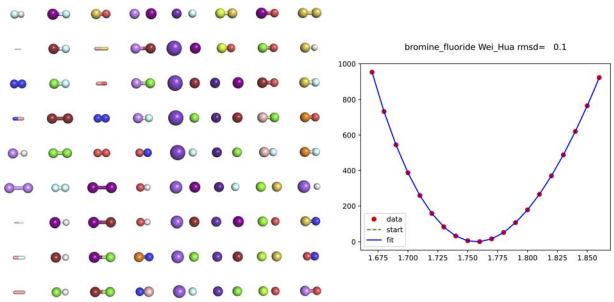
812



Active learning-guided exploration of thermally conductive polymers under strain

Renzheng Zhang, Jiaxin Xu, Hanfeng Zhang, Guoyue Xu and Tengfei Luo*

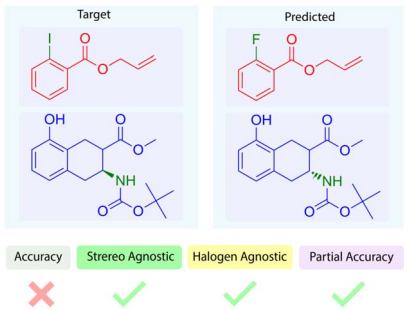
824



Quantitative evaluation of anharmonic bond potentials for molecular simulations

Paul J. van Maaren and David van der Spoel*

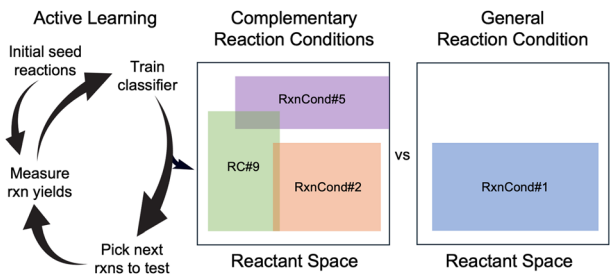
831



Dissecting errors in machine learning for retrosynthesis: a granular metric framework and a transformer-based model for more informative predictions

Arihanth Srikar Tadanki, H. Surya Prakash Rao and U. Deva Priyakumar*

846



Active learning high coverage sets of complementary reaction conditions

Sofia L. Sivilotti, David M. Friday and Nicholas E. Jackson*

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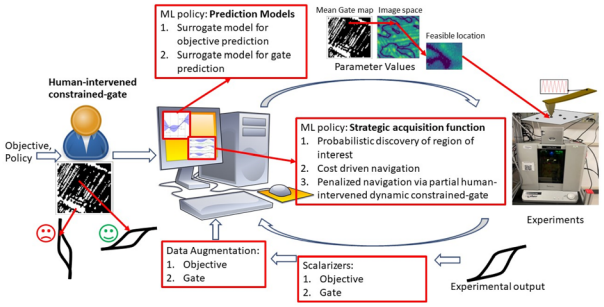
PAPERS

853

SANE: strategic autonomous non-smooth exploration for multiple optima discovery in multi-modal and non-differentiable black-box functions

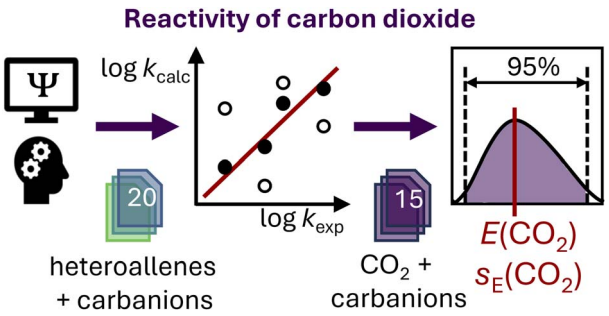
Arpan Biswas, Rama Vasudevan, Rohit Pant, Ichiro Takeuchi, Hiroshi Funakubo and Yongtao Liu



868

Unveiling CO_2 reactivity with data-driven methods

Maike Eckhoff, Kerstin L. Bublitz and Jonny Proppe*



CORRECTION

879

Correction: Distortion/interaction analysis *via* machine learning

Samuel G. Espley, Samuel S. Allsop, David Buttar, Simone Tomasi and Matthew N. Grayson*

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