

Digital Discovery

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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.



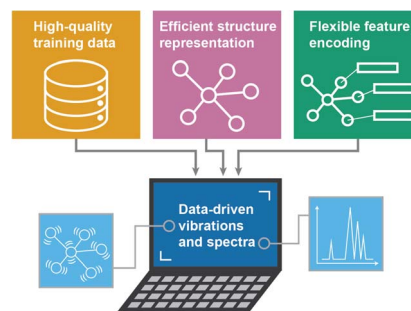
Inside cover
See Linjiang Chen, Fei Zhang, Weiwei Shang, Jun Jiang *et al.*, pp. 636–652. Image reproduced by permission of Jun Jiang from *Digital Discovery*, 2025, 4, 636.

REVIEW

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

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

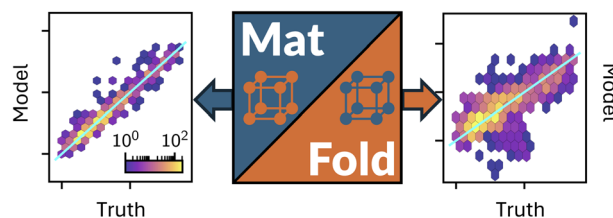


PAPERS

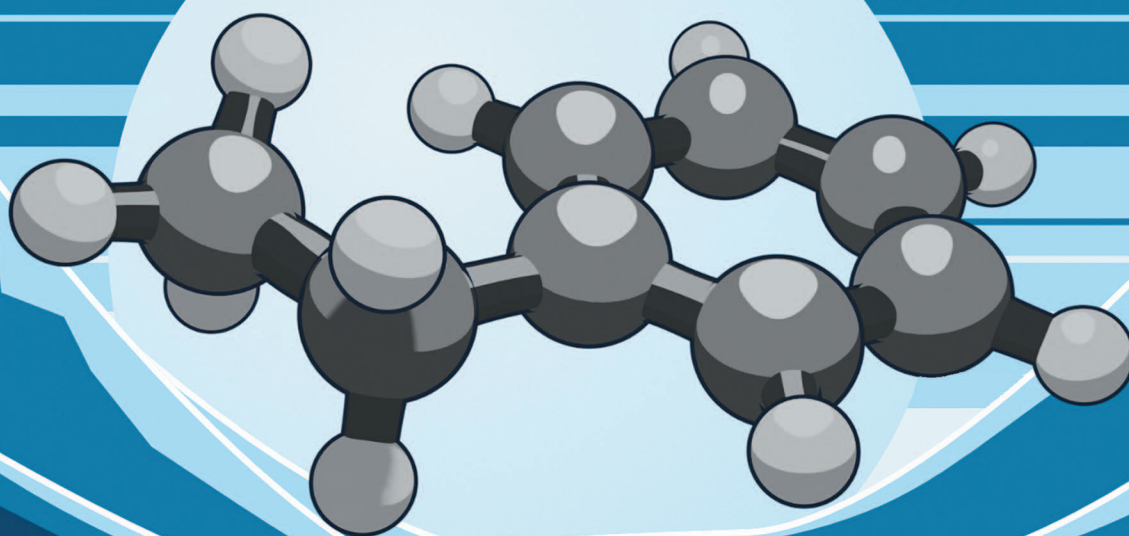
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MatFold: systematic insights into materials discovery models' performance through standardized cross-validation protocols

Matthew D. Witman* and Peter Schindler*



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



September 16th-19th

Zaragoza, Spain · camlcworkshop.github.io



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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*

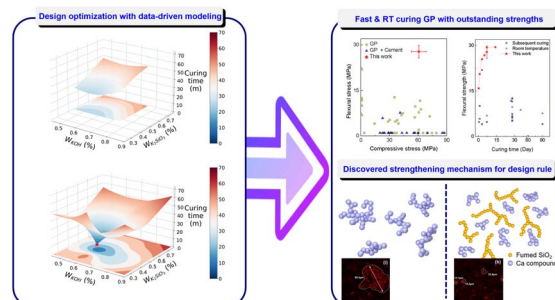


Multi-robot-multi-task

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

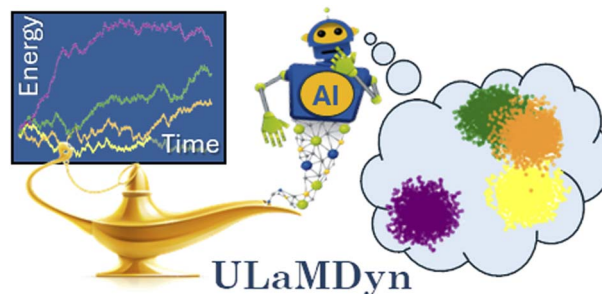
Kyungwon Kim, Hyejeong Song, Sanghun Lee, Hyeongkyu Cho, Hyung Mi Lim and Hyunseok Ko*



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

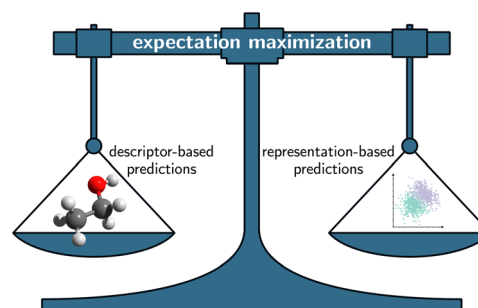
Max Pinheiro Jr,* Matheus de Oliveira Bispo, Rafael S. Mattos, Mariana Telles do Casal, Bidhan Chandra Garain,* Josene M. Toldo, Saikat Mukherjee and Mario Barbatti*



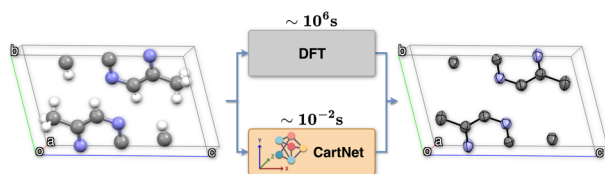
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Balancing molecular information and empirical data in the prediction of physico-chemical properties

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



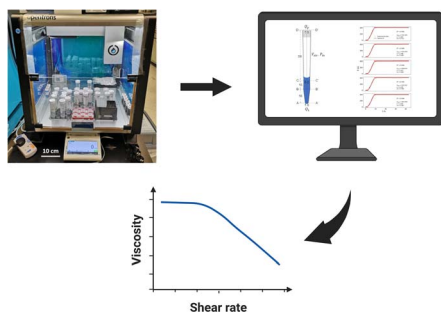
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A Cartesian encoding graph neural network for crystal structure property prediction: application to thermal ellipsoid estimation

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

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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

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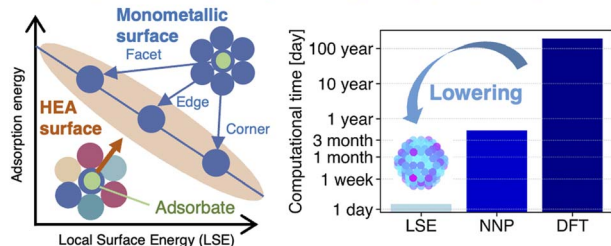


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James R. Deneault, Woojae Kim, Jiseob Kim, Yuzhe Gu, Jorge Chang, Benji Maruyama, Jay I. Myung and Mark A. Pitt*

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Rapid Screening of High-Entropy Alloy (HEA) Catalysts



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

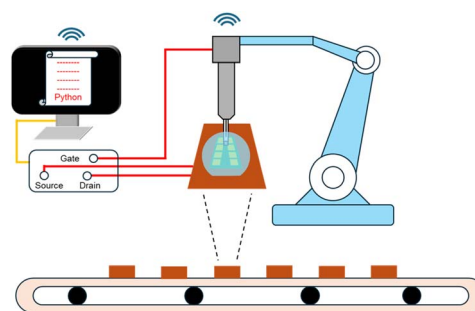
Tomoya Shiota,* Kenji Ishihara and Wataru Mizukami*



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

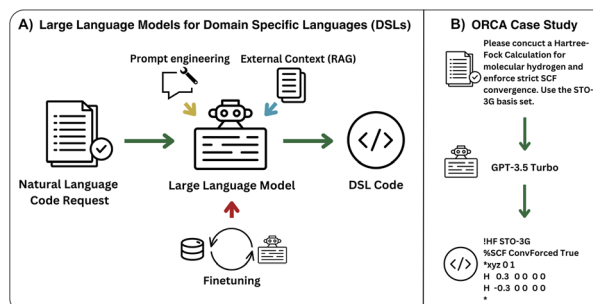
Zhengru Liu, Long Bian, Wenting Shao, Sean I. Hwang and Alexander Star*



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Developing large language models for quantum chemistry simulation input generation

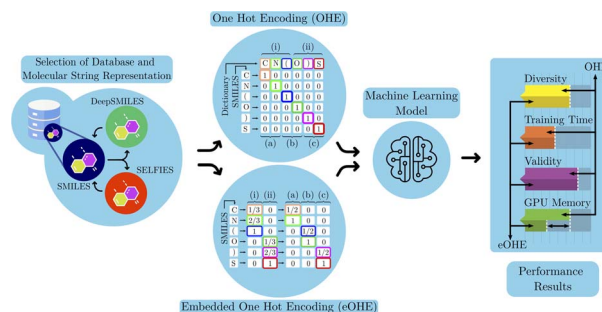
Pieter Floris Jacobs and Robert Pollice*



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

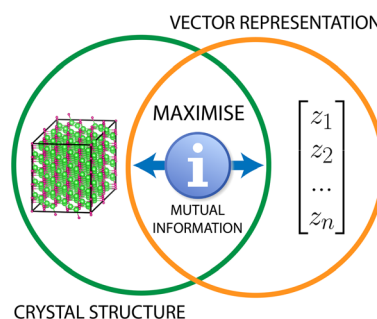
Emilio Nuñez-Andrade,* Isaac Vidal-Daza, James W. Ryan, Rafael Gómez-Bombarelli and Francisco J. Martín-Martínez*



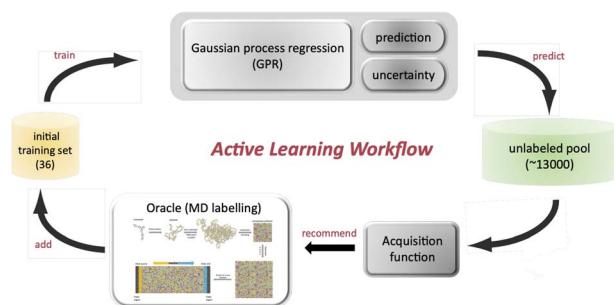
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Establishing Deep InfoMax as an effective self-supervised learning methodology in materials informatics

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



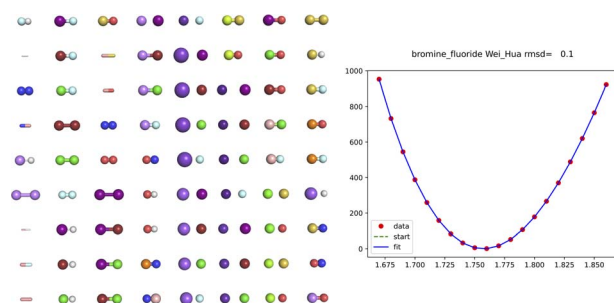
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Active learning-guided exploration of thermally conductive polymers under strain

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

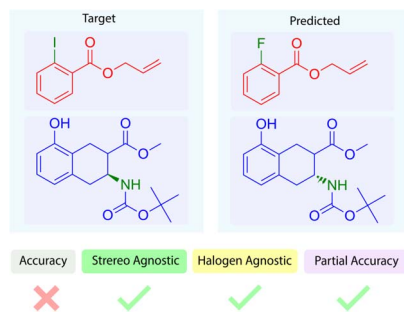
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Quantitative evaluation of anharmonic bond potentials for molecular simulations

Paul J. van Maaren and David van der Spoel*

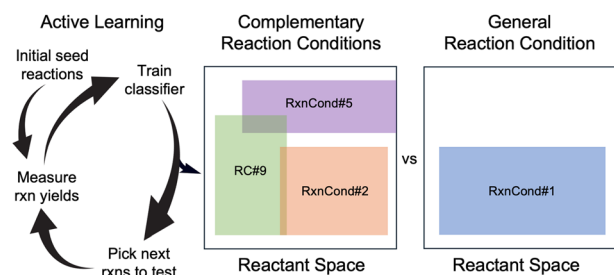
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Arihanth Srikanth Tadanki, H. Surya Prakash Rao and U. Deva Priyakumar*

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Active learning high coverage sets of complementary reaction conditions

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

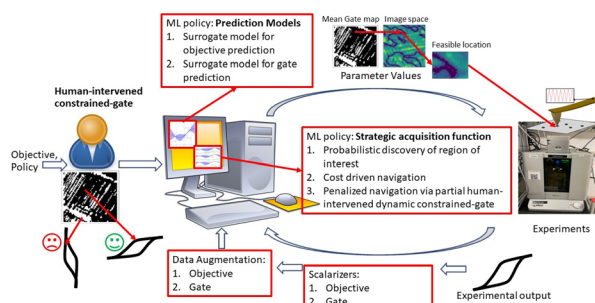


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SANE: strategic autonomous non-smooth exploration for multiple optima discovery in multi-modal and non-differentiable black-box functions

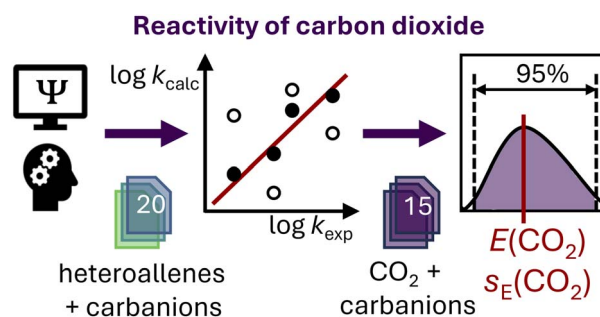
Arpan Biswas, Rama Vasudevan, Rohit Pant, Ichiro Takeuchi, Hiroshi Funakubo and Yongtao Liu



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Maike Eckhoff, Kerstin L. Bublitz and Jonny Proppe*



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Correction: Distortion/interaction analysis via machine learning

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

