Open Access Article. Published on 07 August 2024. Downloaded on 1/22/2026 1:41:21 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

Digital Discovery

rsc.li/digitaldiscovery

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

IN THIS ISSUE

ISSN 2635-098X CODEN DDIIAI 3(8) 1443–1650 (2024)

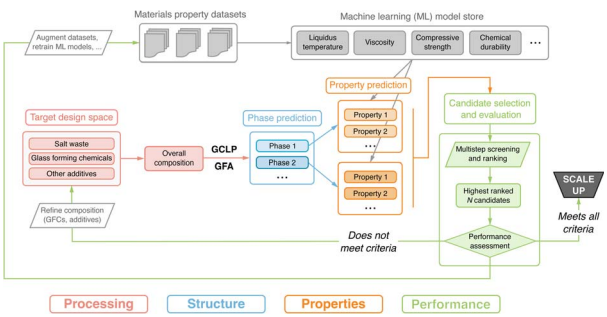
Cover
Yuichiro Chino/Getty Images.

PERSPECTIVE

1450

Towards informatics-driven design of nuclear waste forms

Vinay I. Hegde, Miroslava Peterson, Sarah I. Allec, Xiaonan Lu, Thiruvillamalai Mahadevan, Thanh Nguyen, Jayani Kalahe, Jared Oshiro, Robert J. Seffens, Ethan K. Nickerson, Jincheng Du, Brian J. Riley, John D. Vienna and James E. Saal*

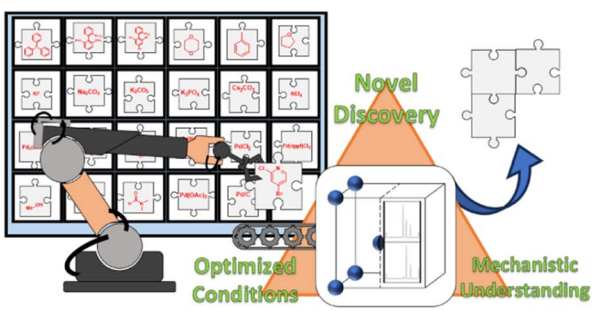


REVIEW

1467

Automated approaches, reaction parameterisation, and data science in organometallic chemistry and catalysis: towards improving synthetic chemistry and accelerating mechanistic understanding

Stuart C. Smith, Christopher S. Horbaczewskyj, Theo F. N. Tanner, Jacob J. Walder and Ian J. S. Fairlamb*



View Article Online

ROYAL SOCIETY OF CHEMISTRY

NEW JOURNAL

RSC Sustainability

GOLD OPEN ACCESS

Dedicated to sustainable chemistry and new solutions

For an open, green and inclusive future

rsc.li/RSCSus

Fundamental questions
Elemental answers

Registered charity number: 207890

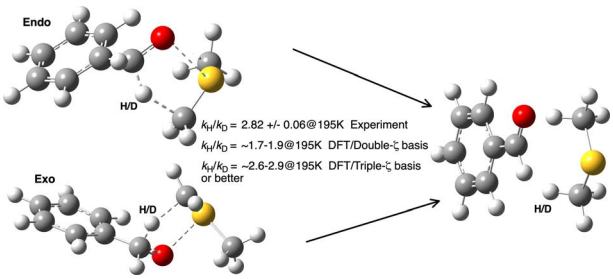
Open Access Article. Published on 07 August 2024. Downloaded on 1/22/2026 1:41:21 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

PAPERS

1496

Modelling kinetic isotope effects for Swern oxidation using DFT-based transition state theory

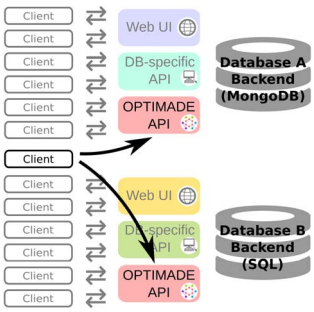
D. Christopher Braddock, Siwoo Lee and Henry S. Rzepa*



1509

Developments and applications of the OPTIMADE API for materials discovery, design, and data exchange

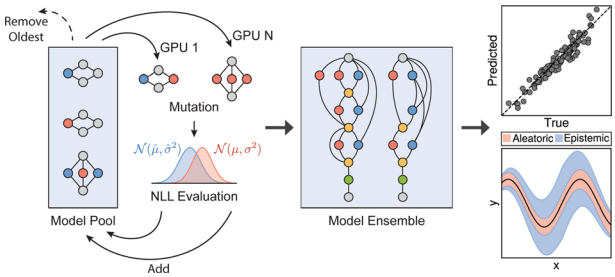
Matthew L. Evans, Johan Bergsma and Andrius Merkys *et al.*



1534

Uncertainty quantification for molecular property predictions with graph neural architecture search

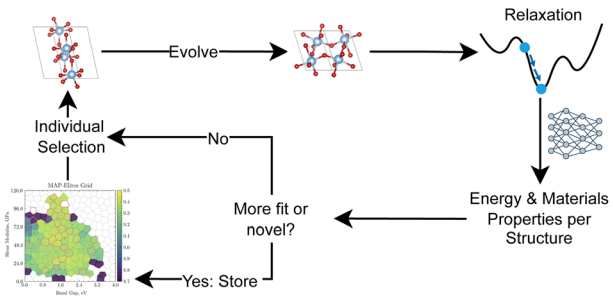
Shengli Jiang,* Shiyi Qin, Reid C. Van Lehn, Prasanna Balaprakash and Victor M. Zavala



1554

Illuminating the property space in crystal structure prediction using Quality-Diversity algorithms

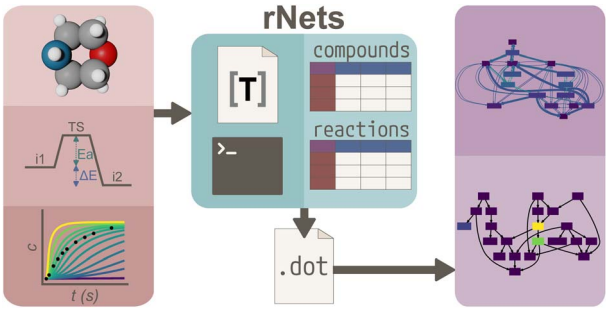
Marta Wolinska,* Aron Walsh and Antoine Cully



Open Access Article. Published on 07 August 2024. Downloaded on 1/22/2026 1:41:21 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

PAPERS

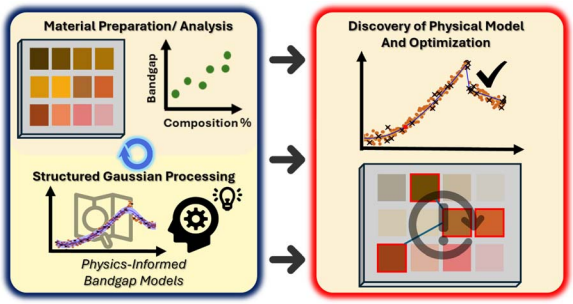
1564



rNets: a standalone package to visualize reaction networks

Sergio Pablo-García,* Raúl Pérez-Soto, Albert Sabadell-Rendón, Diego Garay-Ruiz, Vladyslav Nosylevskyi and Núria López

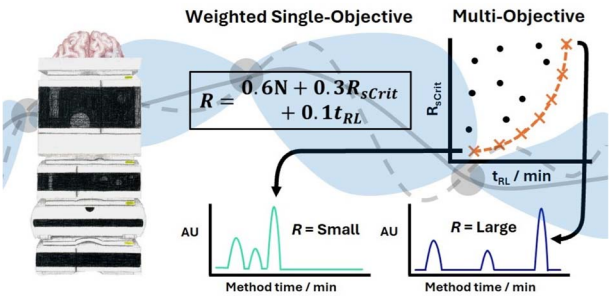
1577



Physics-driven discovery and bandgap engineering of hybrid perovskites

Sheryl L. Sanchez, Elham Foadian, Maxim Ziatdinov, Jonghee Yang, Sergei V. Kalinin, Yongtao Liu* and Mahshid Ahmadi*

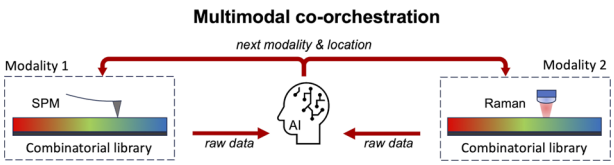
1591



Operator-free HPLC automated method development guided by Bayesian optimization

Thomas M. Dixon, Jeanine Williams, Maximilian Besenhard, Roger M. Howard, James MacGregor, Philip Peach, Adam D. Clayton, Nicholas J. Warren and Richard A. Bourne*

1602



Co-orchestration of multiple instruments to uncover structure–property relationships in combinatorial libraries

Boris N. Slautin,* Utkarsh Pratiush, Ilia N. Ivanov, Yongtao Liu, Rohit Pant, Xiaohang Zhang, Ichiro Takeuchi, Maxim A. Ziatdinov and Sergei V. Kalinin*

This journal is © The Royal Society of Chemistry 2024

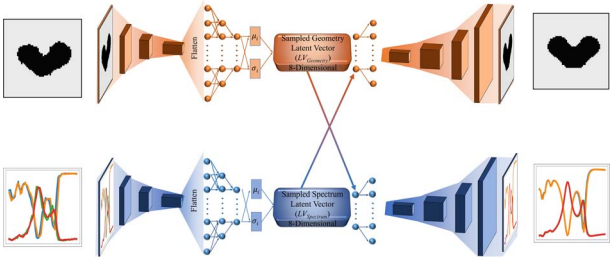
Open Access Article. Published on 07 August 2024. Downloaded on 1/22/2026 1:41:21 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

PAPERS

1612

Deep-learning enabled photonic nanostructure discovery in arbitrarily large shape sets *via* linked latent space representation learning

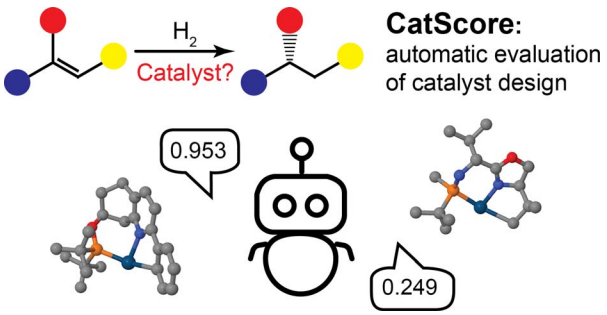
Sudhanshu Singh,* Rahul Kumar,* Soumyashree S. Panda and Ravi S. Hegde



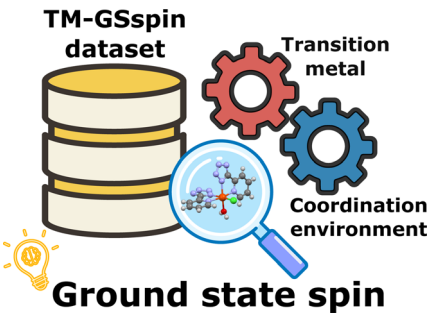
1624

CatScore: evaluating asymmetric catalyst design at high efficiency

Bing Yan* and Kyunghyun Cho



1638

Automated prediction of ground state spin for transition metal complexes

Yuri Cho, Ruben Laplaza, Sergi Vela and Clémence Corminboeuf*