

# Digital Discovery

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## IN THIS ISSUE

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



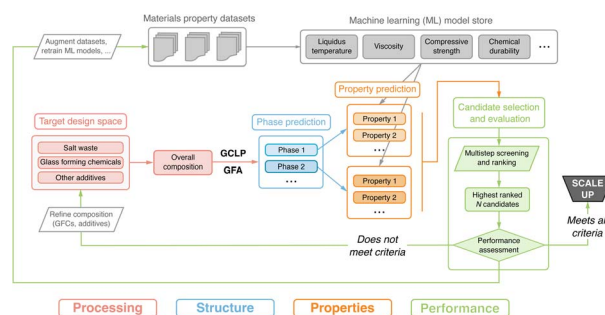
Cover  
Yuichiro Chino/Getty Images.

## 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\*

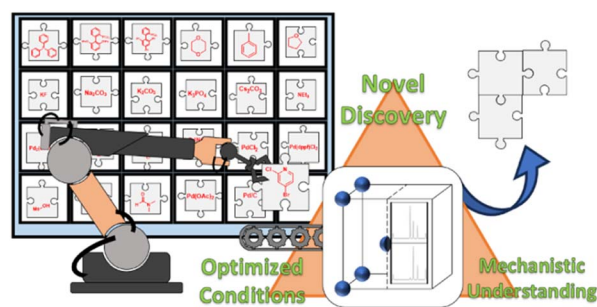


## REVIEW

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### 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\*



# RSC Sustainability

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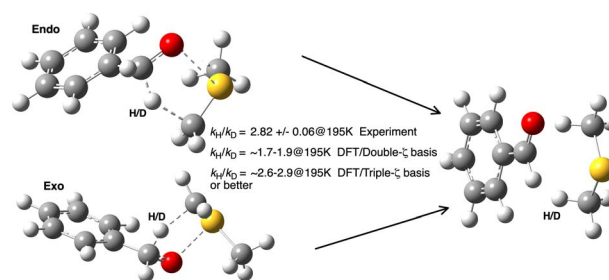
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Fundamental questions  
Elemental answers

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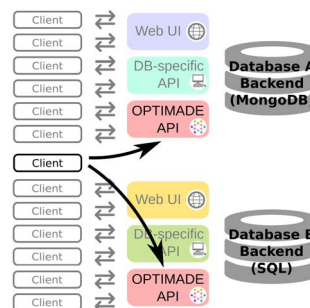
## Modelling kinetic isotope effects for Swern oxidation using DFT-based transition state theory

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



1509

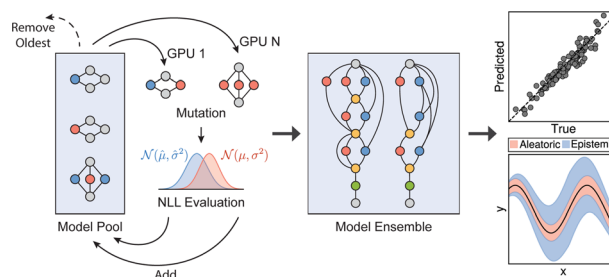
## Developments and applications of the OPTIMADE API for materials discovery, design, and data exchange

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

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## Uncertainty quantification for molecular property predictions with graph neural architecture search

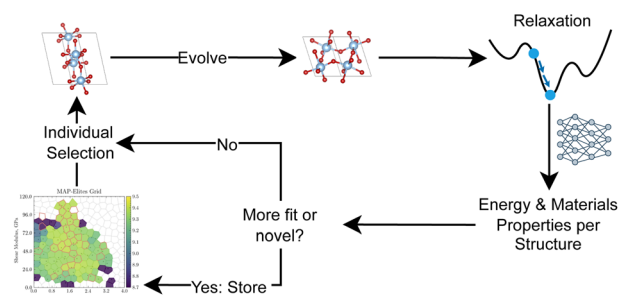
Shengli Jiang,\* Shiyi Qin, Reid C. Van Lehn, Prasanna Balaprakash and Victor M. Zavala



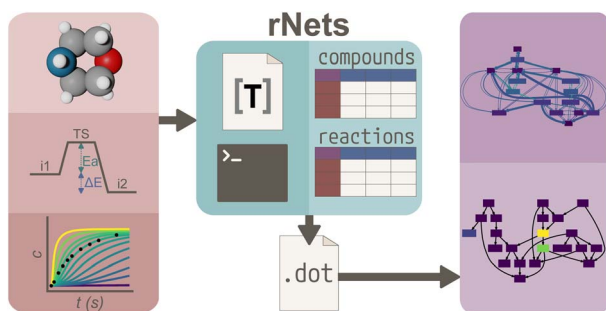
1554

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

Marta Wolinska,\* Aron Walsh and Antoine Cully



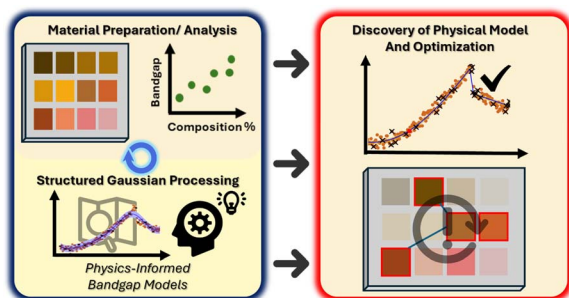
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### rNets: a standalone package to visualize reaction networks

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

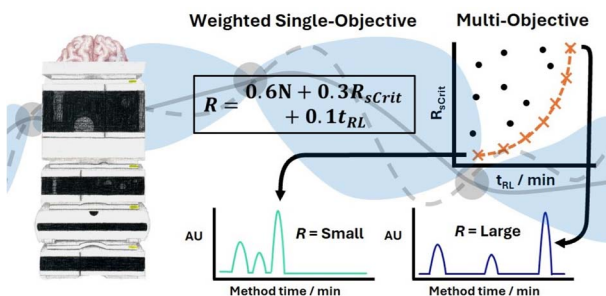
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### Physics-driven discovery and bandgap engineering of hybrid perovskites

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

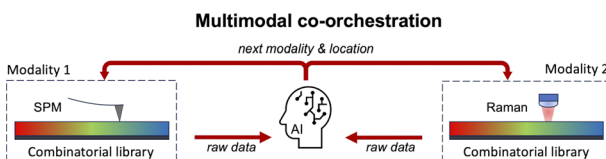
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### Operator-free HPLC automated method development guided by Bayesian optimization

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

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

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

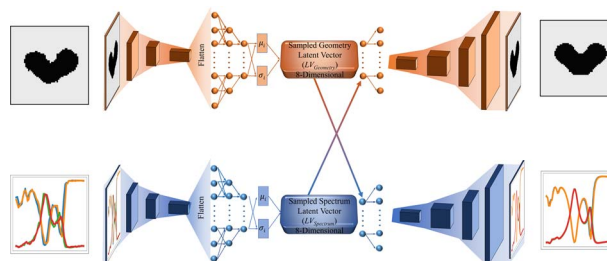


## PAPERS

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

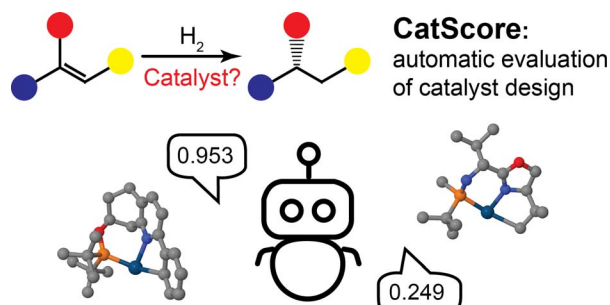
Sudhanshu Singh,\* Rahul Kumar,\* Soumyashree S. Panda and Ravi S. Hegde



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### CatScore: evaluating asymmetric catalyst design at high efficiency

Bing Yan\* and Kyunghyun Cho



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### Automated prediction of ground state spin for transition metal complexes

Yuri Cho, Ruben Laplaza, Sergi Vela and Cl  mence Corminboeuf\*

