Digital Discovery

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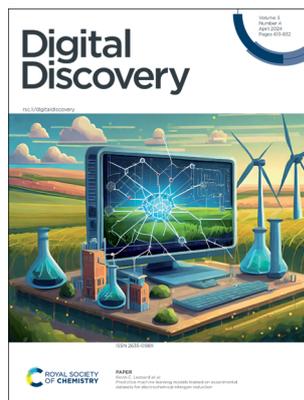
IN THIS ISSUE

PERSPECTIVE

TUTORIAL REVIEW

(a) Study robustness-accuracy tradeoff
(b) Construct ensembles from disparate minima

	Minimum 1	Minimum 2
Loss	low	high
Width	narrow	wide

(c) Feature importance by conserved weights
(d) Parameter selection: Choosing K in K−means

$K=4$ $K=5$ $K=6$

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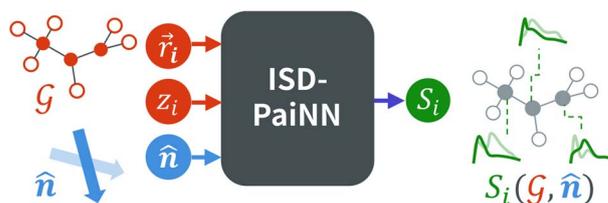## rsc.li/RSCSus

**Fundamental questions
Elemental answers**

COMMUNICATION

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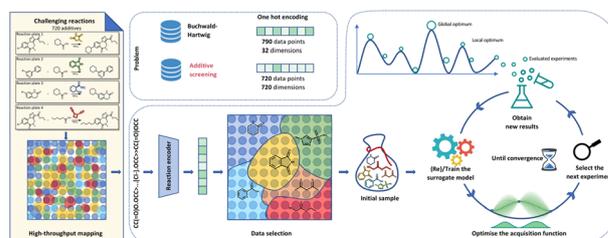
Kiyou Shibata* and Teruyasu Mizoguchi

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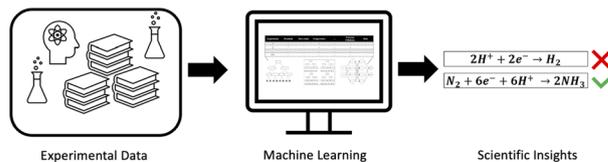
Bojana Ranković,* Ryan-Rhys Griffiths, Henry B. Moss and Philippe Schwaller

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Predictive machine learning models trained on experimental datasets for electrochemical nitrogen reduction
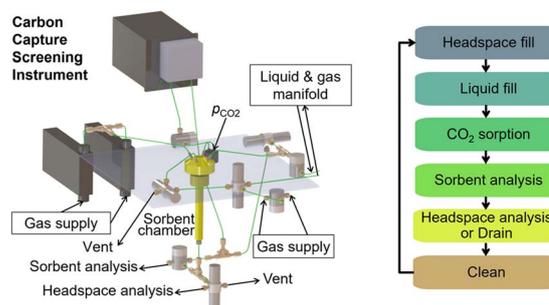
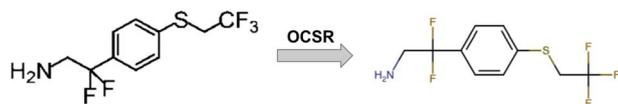Darik A. Rosser, Brianna R. Farris and Kevin C. Leonard*

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Accelerated screening of carbon dioxide capture by liquid sorbents

Ryan J. R. Jones, Yungchieh Lai, Kevin Kan, Dan Guevarra, Joel A. Haber, Natalia M. Ramirez, Alessandra Zito, Clarabella Li, Jenny Y. Yang, Aaron M. Appel and John M. Gregoire*
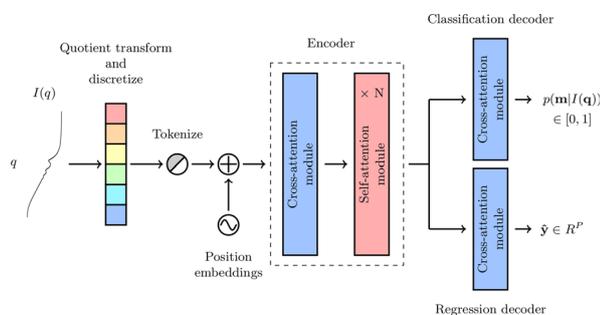
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Comparing software tools for optical chemical structure recognition

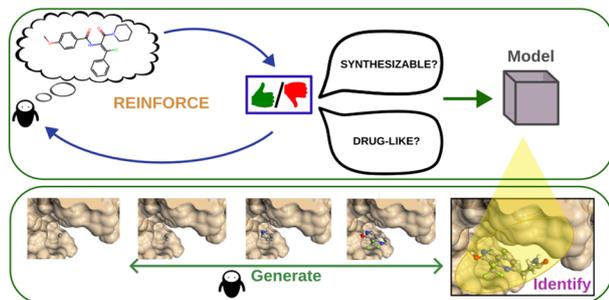Aleksei Krasnov,* Shadrack J. Barnabas, Timo Boehme, Stephen K. Boyer and Lutz Weber*

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Multi-task scattering-model classification and parameter regression of nanostructures from small-angle scattering data

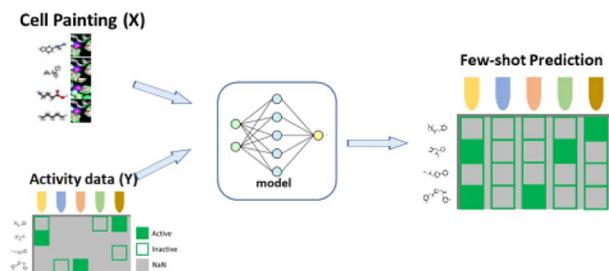Batuhan Yildirim, James Doutch and Jacqueline M. Cole*

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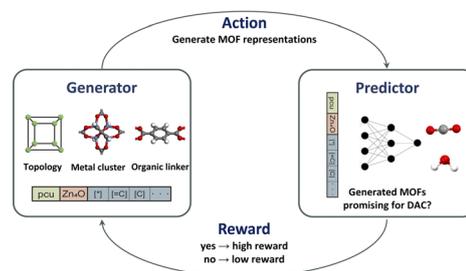
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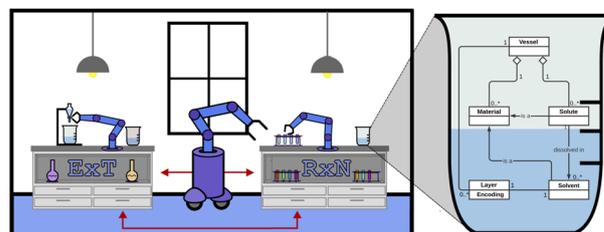
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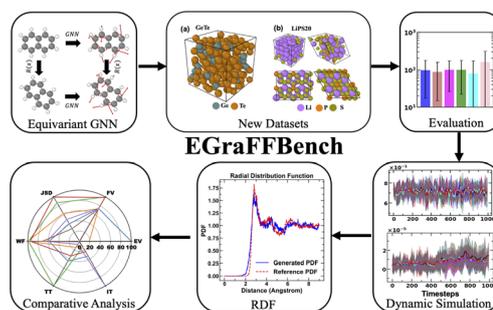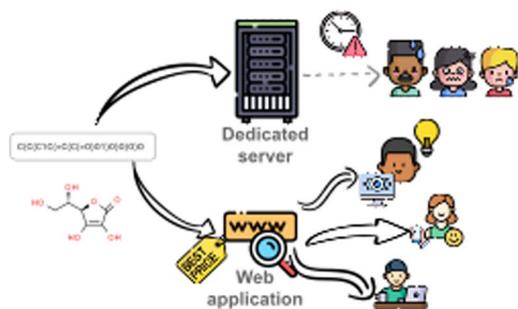
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Learning conditional policies for crystal design using offline reinforcement learning

Prashant Govindarajan,* Santiago Miret, Jarrid Rector-Brooks, Mariano Phielipp, Janarthanan Rajendran and Sarath Chandar
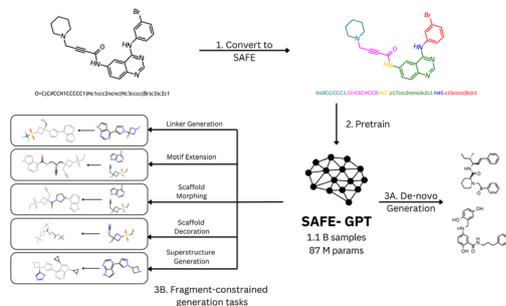
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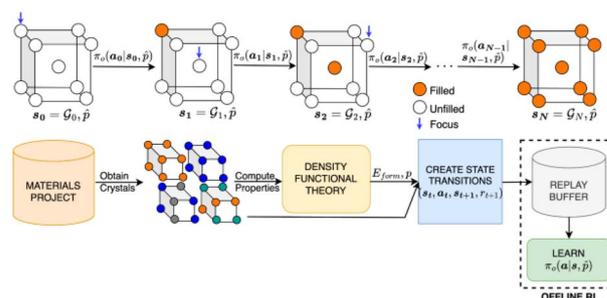
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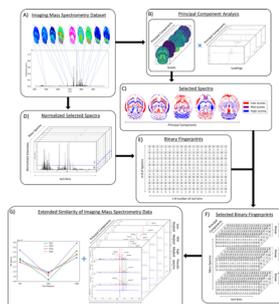
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Gotta be SAFE: a new framework for molecular design

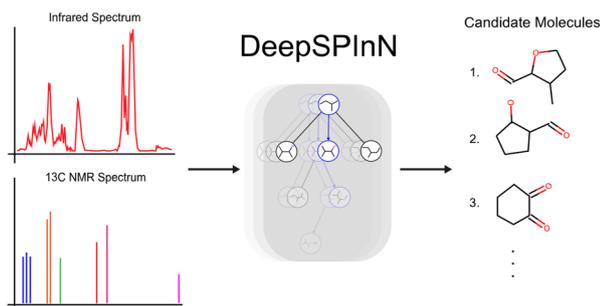Emmanuel Noutahi,* Cristian Gabellini, Michael Craig, Jonathan S. C. Lim and Prudencio Tossou

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Sriram Devata, Bhuvanesh Sridharan, Sarvesh Mehta, Yashaswi Pathak, Siddhartha Laghuvarapu, Girish Varma and U. Deva Priyakumar*