

Digital Discovery

rsc.li/digitaldiscovery

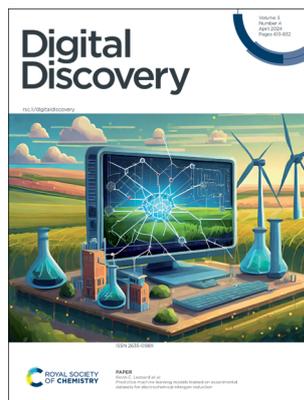
The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

IN THIS ISSUE

ISSN 2635-098X CODEN DDIIAI 3(4) 613–832 (2024)



Cover
See Bojana Ranković, Philippe Schwaller *et al.*, pp. 654–666. Image reproduced by permission of Bojana Ranković from *Digital Discovery*, 2024, 3, 654. Image created using Adobe Firefly.



Inside cover
See Kevin C. Leonard *et al.*, pp. 667–673. Image reproduced by permission of Kevin C. Leonard from *Digital Discovery*, 2024, 3, 667. Image created using Adobe Firefly.

PERSPECTIVE

621

The future of self-driving laboratories: from human in the loop interactive AI to gamification

Holland Hysmith, Elham Foadian, Shakti P. Padhy, Sergei V. Kalinin, Rob G. Moore, Olga S. Ovchinnikova and Mahshid Ahmadi*

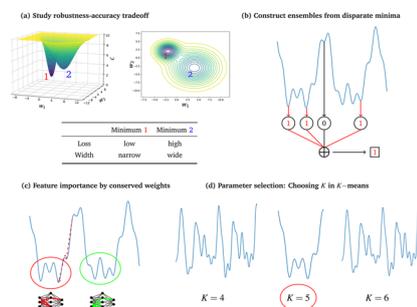


TUTORIAL REVIEW

637

Insights into machine learning models from chemical physics: an energy landscapes approach (EL for ML)

Maximilian P. Niroomand, Luke Dicks, Edward O. Pyzer-Knapp* and David J. Wales*



RSC Sustainability

GOLD
OPEN
ACCESS

Dedicated to sustainable
chemistry and new solutions

For an open, green and inclusive future

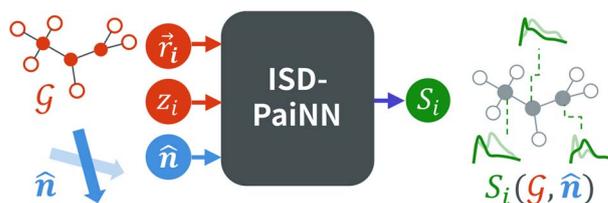
rsc.li/RSCSus

Fundamental questions
Elemental answers

649

A message passing neural network for predicting dipole moment dependent core electron excitation spectra

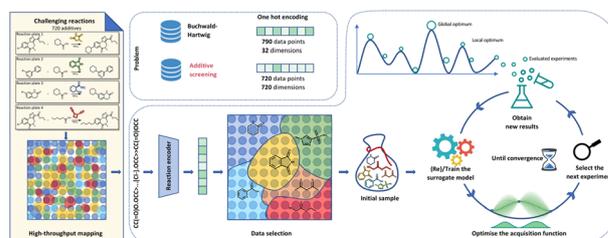
Kiyou Shibata* and Teruyasu Mizoguchi



654

Bayesian optimisation for additive screening and yield improvements – beyond one-hot encoding

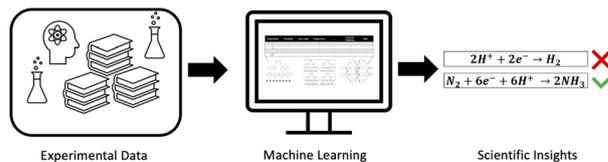
Bojana Ranković,* Ryan-Rhys Griffiths, Henry B. Moss and Philippe Schwaller



667

Predictive machine learning models trained on experimental datasets for electrochemical nitrogen reduction

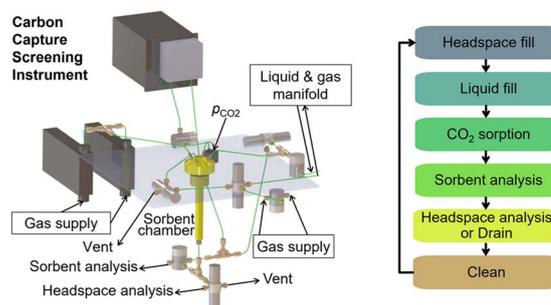
Darik A. Rosser, Brianna R. Farris and Kevin C. Leonard*



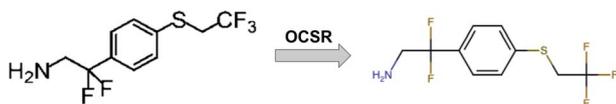
674

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*



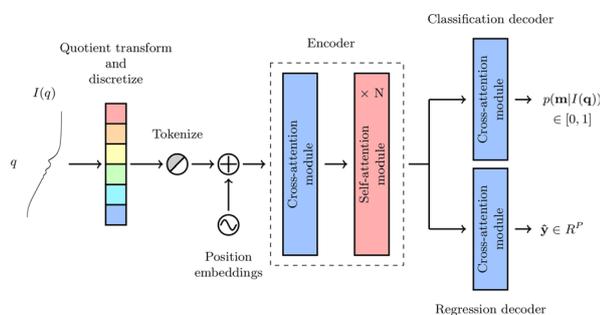
681



Comparing software tools for optical chemical structure recognition

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

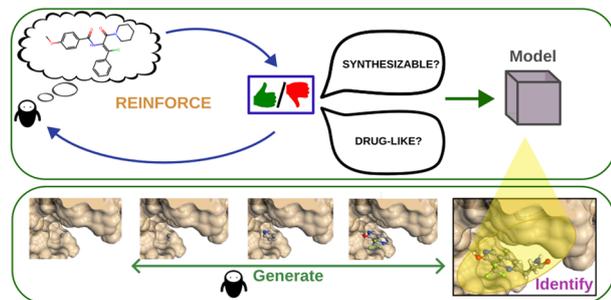
694



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

Batuhan Yildirim, James Douth and Jacqueline M. Cole*

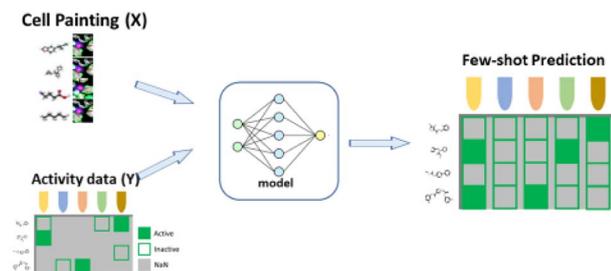
705



SPOTLIGHT: structure-based prediction and optimization tool for ligand generation on hard-to-drug targets – combining deep reinforcement learning with physics-based *de novo* drug design

Venkata Sai Sreyas Adury and Arnab Mukherjee*

719



FSL-CP: a benchmark for small molecule activity few-shot prediction using cell microscopy images

Son V. Ha, Lucas Leuschner and Paul Czodrowski*

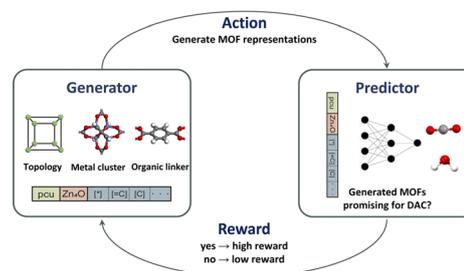


728

Inverse design of metal–organic frameworks for direct air capture of CO₂ via deep reinforcement learning

Hyunsoo Park, Sauradeep Majumdar, Xiaoqi Zhang, Jihan Kim* and Berend Smit*

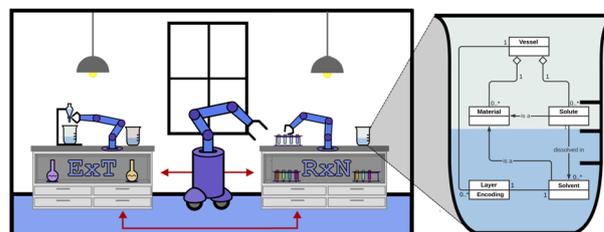
Reinforcement Learning Framework for DAC



742

ChemGymRL: A customizable interactive framework for reinforcement learning for digital chemistry

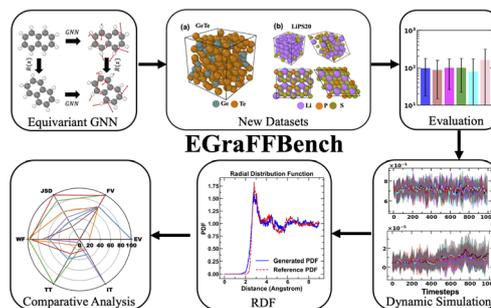
Chris Beeler, Sriram Ganapathi Subramanian, Kyle Sprague, Mark Baula, Nouha Chatti, Amanuel Dawit, Xinkai Li, Nicholas Paquin, Mitchell Shahan, Zihan Yang, Colin Bellinger, Mark Crowley* and Isaac Tamblyn



759

EGraFFBench: evaluation of equivariant graph neural network force fields for atomistic simulations

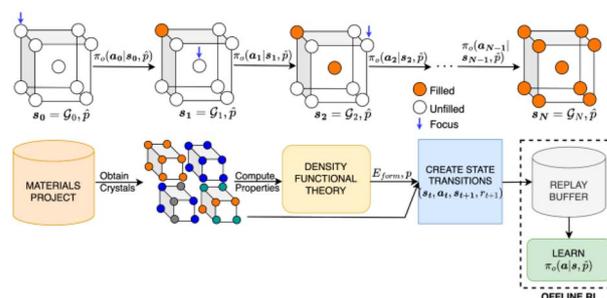
Vaibhav Bihani, Sajid Mannan, Utkarsh Pratiush, Tao Du, Zhimin Chen, Santiago Miret, Matthieu Micoulaut, Morten M. Smedskjaer, Sayan Ranu* and N. M. Anoop Krishnan*



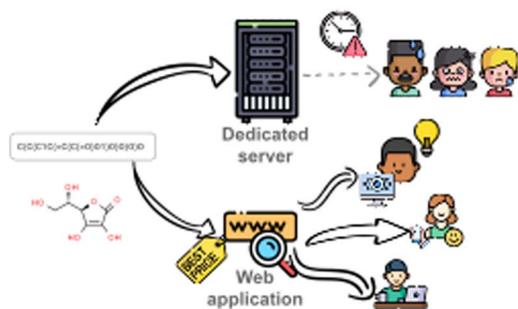
769

Learning conditional policies for crystal design using offline reinforcement learning

Prashant Govindarajan,* Santiago Miret, Jarrid Rector-Brooks, Mariano Phielipp, Janarthanan Rajendran and Sarath Chandar



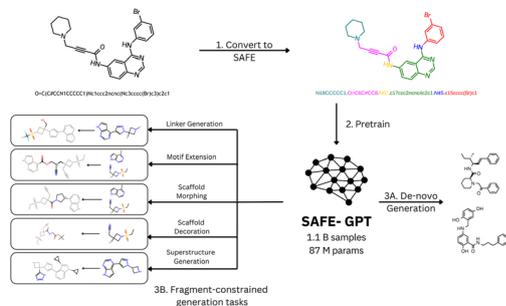
786



Predicting small molecules solubility on endpoint devices using deep ensemble neural networks

Mayk Caldas Ramos and Andrew D. White*

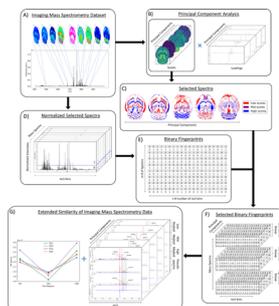
796



Gotta be SAFE: a new framework for molecular design

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

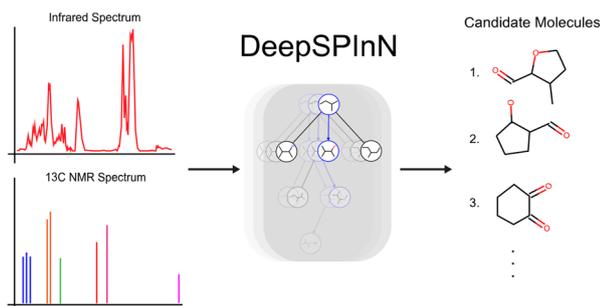
805



Extended similarity methods for efficient data mining in imaging mass spectrometry

Nicholas R. Ellin, Yingchan Guo, Ramón Alain Miranda-Quintana* and Boone M. Prentice*

818



DeepSPINN – deep reinforcement learning for molecular structure prediction from infrared and ^{13}C NMR spectra

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

