

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 2(5) 1221–1632 (2023)



Cover
See Ryan C. Fortenberry *et al.*, pp. 1269–1288.
Image reproduced by permission of Ryan C. Fortenberry from *Digital Discovery*, 2023, 2, 1269.



Inside cover
See Jean-Louis Reymond *et al.*, pp. 1289–1296. Image reproduced by permission of Markus Orsi from *Digital Discovery*, 2023, 2, 1289.
Background: David Teniers the Younger, "The Alchemist". Mauritshuis, The Hague.

PERSPECTIVES

1233

14 examples of how LLMs can transform materials science and chemistry: a reflection on a large language model hackathon

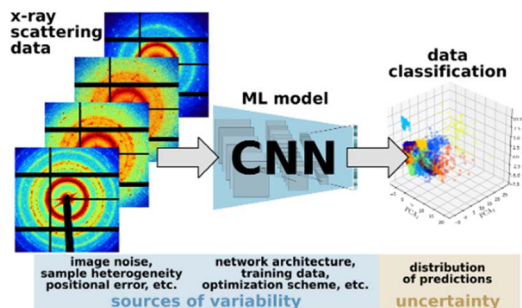
K. M. Jablonka,* Q. Ai, A. Al-Feghali, S. Badhwar, J. D. Bocarsly, A. M. Bran, S. Bringuier, L. C. Brinson, K. Choudhary, D. Circi, S. Cox, W. A. de Jong, M. L. Evans, N. Gastellu, J. Genzling, M. V. Gil, A. K. Gupta, Z. Hong, A. Imran, S. Kruschwitz, A. Labarre, J. Lála, T. Liu, S. Ma, S. Majumdar, G. W. Merz, N. Moitessier, E. Moubarak, B. Mouriño, B. Pelkie, M. Pieler, M. Ramos, B. Ranković, S. G. Rodrigues, J. N. Sanders, P. Schwaller, M. Schwarting, J. Shi, B. Smit, B. E. Smith, J. Van Herck, C. Völker, L. Ward, S. Warren, B. Weiser, S. Zhang, X. Zhang, G. A. Zia, A. Scourtas, K. J. Schmidt, I. Foster, A. D. White and B. Blaiszik*



1251

A rigorous uncertainty-aware quantification framework is essential for reproducible and replicable machine learning workflows

Line Pouchard, Kristofer G. Reyes, Francis J. Alexander and Byung-Jun Yoon*



Editorial Staff

Editor

Anna Rulka

Deputy Editor

Audra Taylor

Editorial Production Manager

Viktoria Titmus

Assistant Editors

Shwetha Krishna, Angelica-Jane Onyekwere, Michael Whitelaw, Alexander Whiteside

Editorial Assistant

Samantha Campos

Publishing Assistant

Brittany Hanlon

Publisher

Neil Hammond

For queries about submitted articles please contact Viktoria Titmus, Editorial Production Manager in the first instance. E-mail digitaldiscovery@rsc.org

For pre-submission queries please contact Anna Rulka, Editor.

Email digitaldiscovery-rsc@rsc.org

Digital Discovery (electronic: ISSN 2635-098X) is published 6 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, UK CB4 0WF.

Digital Discovery is a Gold Open Access journal and all articles are free to read. Please email orders@rsc.org to register your interest or contact Royal Society of Chemistry Order Department, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK Tel +44 (0)1223 432398; E-mail: orders@rsc.org

Whilst this material has been produced with all due care, the Royal Society of Chemistry cannot be held responsible or liable for its accuracy and completeness, nor for any consequences arising from any errors or the use of the information contained in this publication. The publication of advertisements does not constitute any endorsement by the Royal Society of Chemistry or Authors of any products advertised. The views and opinions advanced by contributors do not necessarily reflect those of the Royal Society of Chemistry which shall not be liable for any resulting loss or damage arising as a result of reliance upon this material. The Royal Society of Chemistry is a charity, registered in England and Wales, Number 207890, and a company incorporated in England by Royal Charter (Registered No. RC000524), registered office: Burlington House, Piccadilly, London W1J 0BA, UK, Telephone: +44 (0) 207 4378 6556.

Advertisement sales:

Tel +44 (0) 1223 432246; Fax +44 (0) 1223 426017;

E-mail advertising@rsc.org

For marketing opportunities relating to this journal,

contact marketing@rsc.org

Digital Discovery

rsc.li/digitaldiscovery

Digital Discovery is a gold open access journal publishing top research at the intersection of chemistry, materials science and biotechnology. Blurring the barriers between computation and experimentation, we focus on the integration of digital and automation tools with science, putting data first to ensure reproducibility and faster progress.

Editorial Board

Editor in Chief

Alán Aspuru-Guzik, University of Toronto, Canada

Associate Editors

Jason E. Hein, University of British Columbia, Canada

Linda Hung, Toyota Research Institute, USA

Joshua Schrier, Fordham University, USA

Kedar Hippalgaonkar, Nanyang Technological University, Singapore

Cesar de la Fuente, University of Pennsylvania, USA

Members

Yousung Jung, KAIST, South Korea

Anat Milo, Ben-Gurion University of the

Negev, Israel

Lilo D. Pozzo, University of Washington, USA

Ekaterina Skorb, ITMO University, Russia

Advisory Board

Juan Alegre, Colorado State University, USA
Silvana Botti, Friedrich Schiller University Jena, Germany

Pablo Carbonell, University of Valencia, Spain

Cecilia Clementi, Freie Universität Berlin, Germany

Conor Coley, MIT, USA

Abigail Doyle, University of California Los Angeles, USA

Ola Engkvist, AstraZeneca and Chalmers

University of Technology, Sweden

Ian Foster, University of Chicago, USA

Jan Jensen, University of Copenhagen, Denmark

Heather Kulik, MIT, USA

Shuye Ping Ong, University of California San Diego, USA

Marwin Segler, Microsoft, Germany

Berend Smit, EPFL, Switzerland

Isao Tanaka, Kyoto University, Japan

Alexandre Tkatchenko, University of

Luxembourg, Luxembourg

Koji Tsuda, The University of Tokyo, Japan

Information for Authors

Full details on how to submit material for publication in Digital Discovery are given in the instructions for Authors (available from <http://www.rsc.org/authors>). Submissions should be made via the journal's homepage: rsc.li/digitaldiscovery

Authors may reproduce/republish portions of their published contribution without seeking permission from the Royal Society of Chemistry, provided that any such republication is accompanied by an acknowledgement in the form: (Original Citation)–Reproduced by permission of the Royal Society of Chemistry.

This journal is © The Royal Society of Chemistry 2023.

Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulation 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the Publishers or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

Registered charity number: 207890

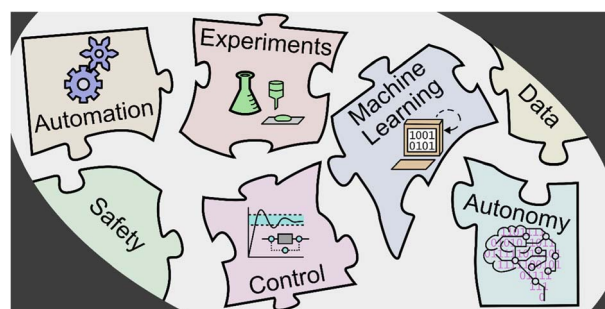


PERSPECTIVES

1259

Integrating autonomy into automated research platforms

Richard B. Canty, Brent A. Koscher, Matthew A. McDonald and Klavs F. Jensen*

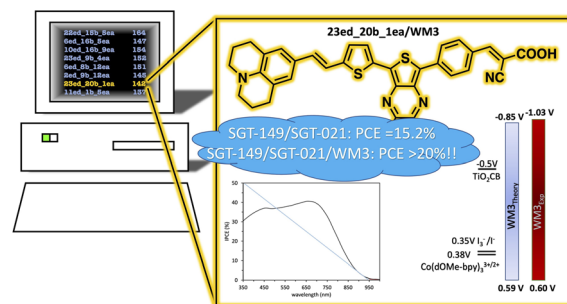


PAPERS

1269

An automated quantum chemistry-driven, experimental characterization for high PCE donor- π -acceptor NIR molecular dyes

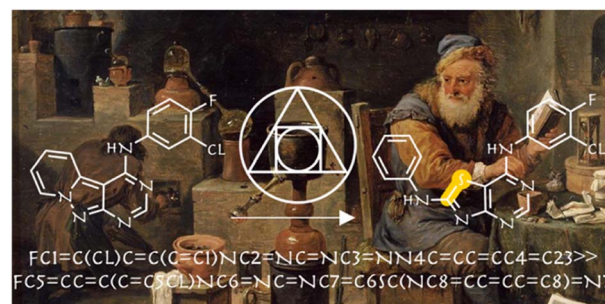
Taylor J. Santaloci, William E. Meador, Austin M. Wallace, E. Michael Valencia, Blake N. Rogers, Jared H. Delcamp and Ryan C. Fortenberry*



1289

Alchemical analysis of FDA approved drugs

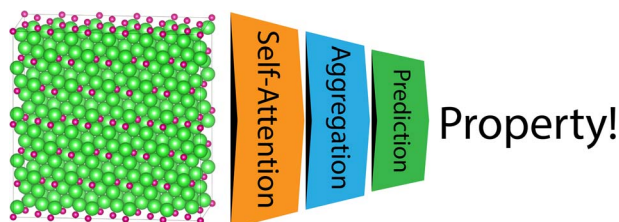
Markus Orsi, Daniel Probst, Philippe Schwaller and Jean-Louis Reymond*



1297

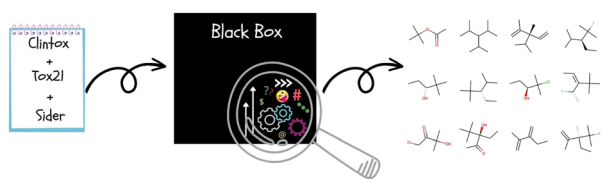
Site-Net: using global self-attention and real-space supercells to capture long-range interactions in crystal structures

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



PAPERS

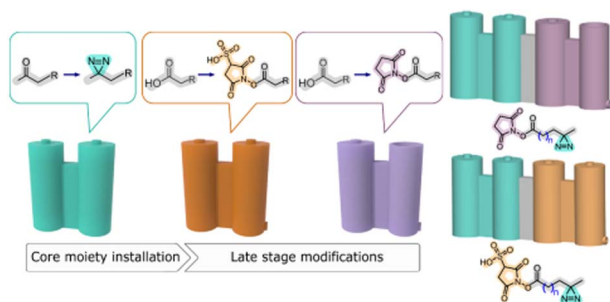
1311



Generating structural alerts from toxicology datasets using the local interpretable model-agnostic explanations method

Cayque Monteiro Castro Nascimento, Paloma Guimarães Moura and Andre Silva Pimentel*

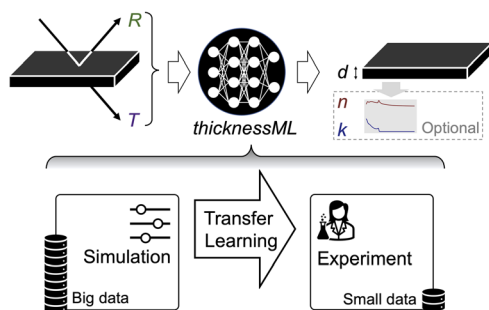
1326



Digital design and 3D printing of reactionware for on demand synthesis of high value probes

Przemyslaw Frei, Philip J. Kitson, Alexander X. Jones and Leroy Cronin*

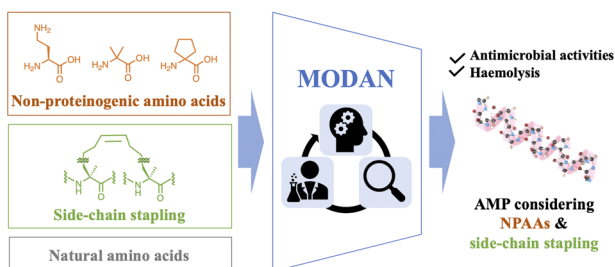
1334



Tackling data scarcity with transfer learning: a case study of thickness characterization from optical spectra of perovskite thin films

Siyu Isaac Parker Tian, Zekun Ren, Selvaraj Venkataraj, Yuanhang Cheng, Daniil Bash, Felipe Oviedo, J. Senthilnath, Vijila Chellappan, Yee-Fun Lim, Armin G. Aberle, Benjamin P. MacLeod, Fraser G. L. Parlane, Curtis P. Berlinguette, Qianxiao Li, Tonio Buonassisi* and Zhe Liu

1347



Design of antimicrobial peptides containing non-proteinogenic amino acids using multi-objective Bayesian optimisation

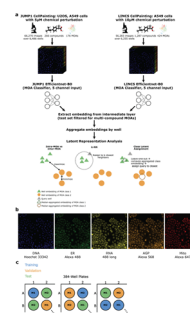
Yuki Murakami, Shoichi Ishida, Yosuke Demizu and Kei Terayama*



1354

Deep representation learning determines drug mechanism of action from cell painting images

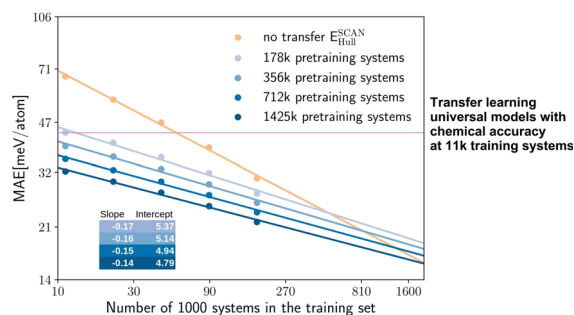
Daniel R. Wong,* David J. Logan, Santosh Hariharan, Robert Stanton, Djork-Arné Clevert and Andrew Kiruluta



1368

Transfer learning on large datasets for the accurate prediction of material properties

Noah Hoffmann, Jonathan Schmidt, Silvana Botti and Miguel A. L. Marques*

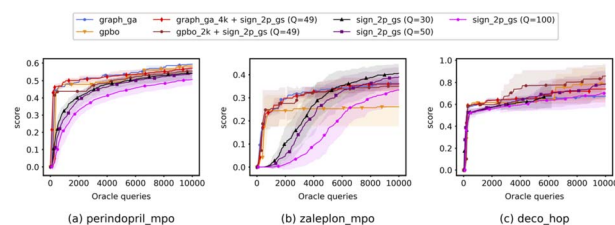


Transfer learning universal models with chemical accuracy at 11k training systems

1380

Understanding and improving zeroth-order optimization methods on AI-driven molecule optimization

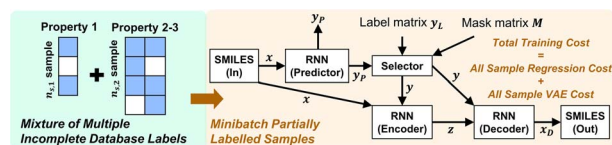
Elvin Lo and Pin-Yu Chen*



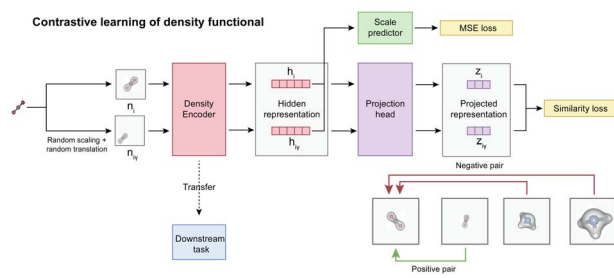
1390

Multi-constraint molecular generation using sparsely labelled training data for localized high-concentration electrolyte diluent screening

Jonathan P. Mailoa,* Xin Li, Jiezhong Qiu and Shengyu Zhang*



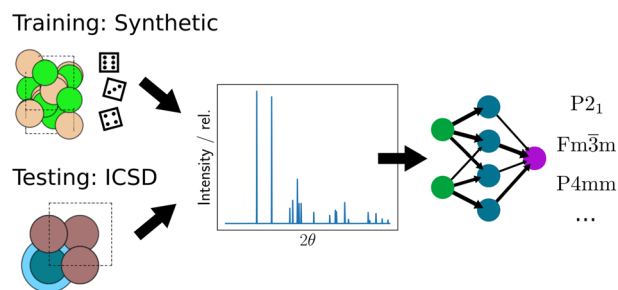
1404



Incorporation of density scaling constraint in density functional design via contrastive representation learning

Weiyi Gong, Tao Sun, Hexin Bai, Shah Tanvir ur Rahman Chowdhury, Peng Chu, Anoj Aryal, Jie Yu, Haibin Ling,* John P. Perdew* and Qimin Yan*

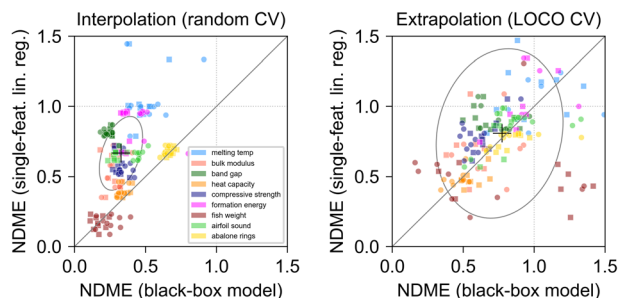
1414



Neural networks trained on synthetically generated crystals can extract structural information from ICSD powder X-ray diffractograms

Henrik Schopmans, Patrick Reiser and Pascal Friederich*

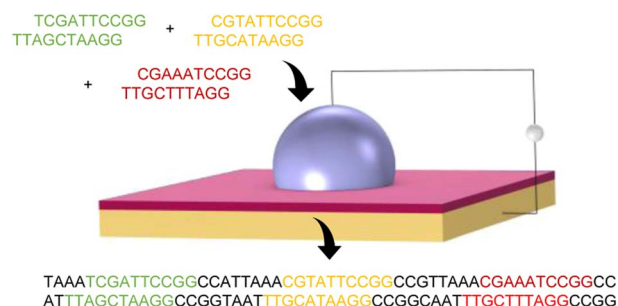
1425



Interpretable models for extrapolation in scientific machine learning

Eric S. Muckley, James E. Saal,* Bryce Meredig, Christopher S. Roper and John H. Martin

1436



Automated routing of droplets for DNA storage on a digital microfluidics platform

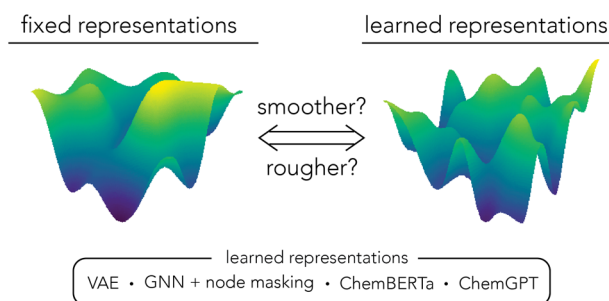
Ajay Manicka, Andrew Stephan, Sriram Chari, Gemma Mendonsa, Peyton Okubo, John Stolzberg-Schray, Anil Reddy and Marc Riedel



1452

Evaluating the roughness of structure–property relationships using pretrained molecular representations

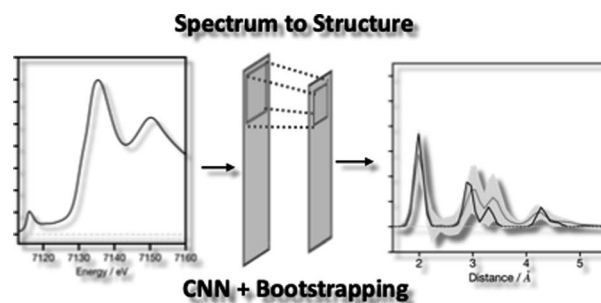
David E. Graff, Edward O. Pyzer-Knapp, Kirk E. Jordan, Eugene I. Shakhnovich and Connor W. Coley



1461

Towards the automated extraction of structural information from X-ray absorption spectra

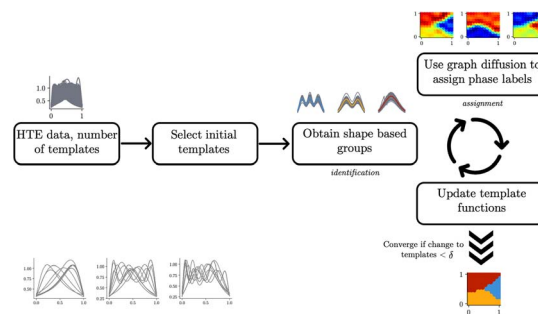
Tudur David,* Nik Khadijah Nik Aznan, Kathryn Garside and Thomas Penfold



1471

Metric geometry tools for automatic structure phase map generation

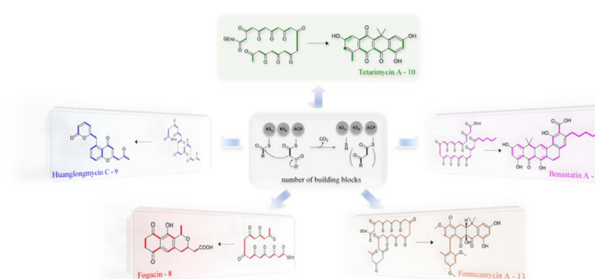
Kiran Vaddi,* Karen Li and Lilo D. Pozzo



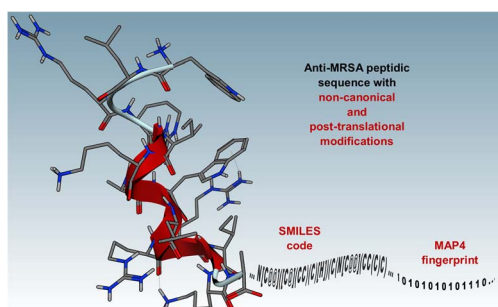
1484

A deep learning model for type II polyketide natural product prediction without sequence alignment

Jiaquan Huang, Qiandi Gao, Ying Tang, Yaxin Wu, Heqian Zhang* and Zhiwei Qin*



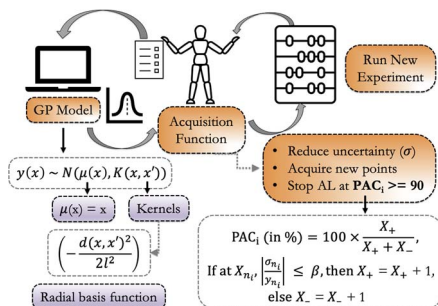
1494



Mapping the structure–activity landscape of non-canonical peptides with MAP4 fingerprinting

Edgar López-López,^{*} Oscar Robles, Fabien Plisson and José L. Medina-Franco^{*}

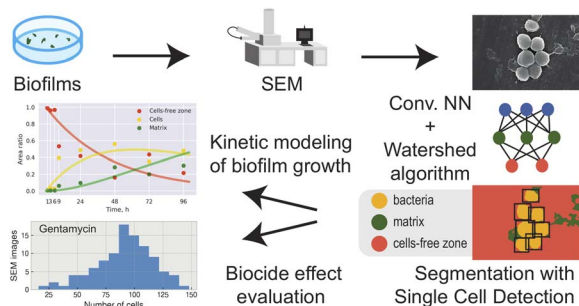
1506



Active learning for efficient navigation of multi-component gas adsorption landscapes in a MOF

Krishnendu Mukherjee, Etinosa Osaro and Yamil J. Colón^{*}

1522



Digital biology approach for macro-scale studies of biofilm growth and biocide effects with electron microscopy

Konstantin S. Kozlov, Daniil A. Boiko, Elena V. Detusheva, Konstantin V. Detushev, Evgeniy O. Pentsak, Anatoly N. Vereshchagin and Valentine P. Ananikov^{*}

1540



Go with the flow: deep learning methods for autonomous viscosity estimations

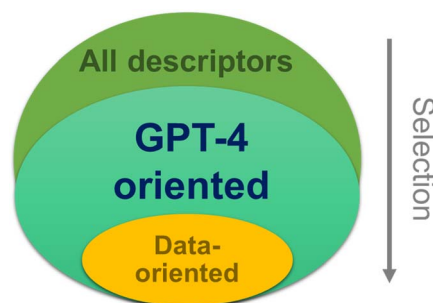
Michael Walker, Gabriella Pizzuto, Hatem Fakhrudeen and Andrew I. Cooper^{*}



1548

Using GPT-4 in parameter selection of polymer informatics: improving predictive accuracy amidst data scarcity and 'Ugly Duckling' dilemma

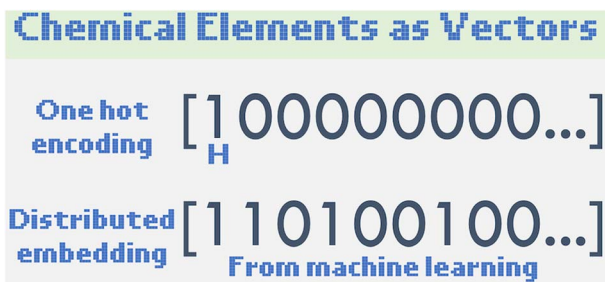
Kan Hatakeyama-Sato,* Seigo Watanabe, Naoki Yamane, Yasuhiko Igarashi and Kenichi Oyaizu*



1558

Element similarity in high-dimensional materials representations

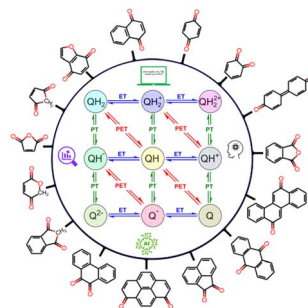
Anthony Onwuli, Ashish V. Hegde, Kevin V. T. Nguyen, Keith T. Butler* and Aron Walsh*



1565

Density functional theory and machine learning for electrochemical square-scheme prediction: an application to quinone-type molecules relevant to redox flow batteries

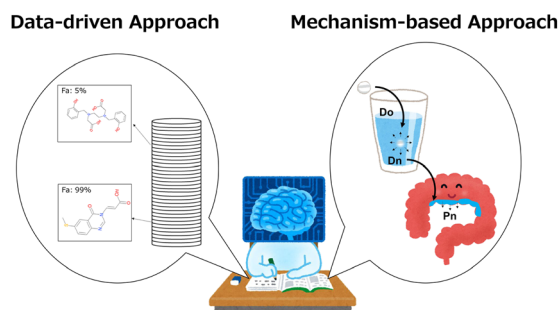
Arsalan Hashemi,* Reza Khakpour, Amir Mahdian, Michael Busch, Pekka Peljo and Kari Laasonen



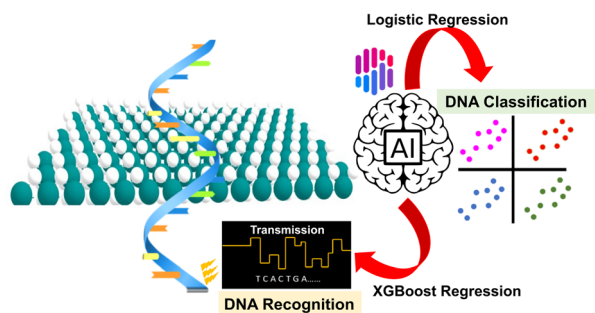
1577

Combined data-driven and mechanism-based approaches for human-intestinal-absorption prediction in the early drug-discovery stage

Koichi Handa,* Sakae Sugiyama, Michiharu Kageyama and Takeshi Iijima



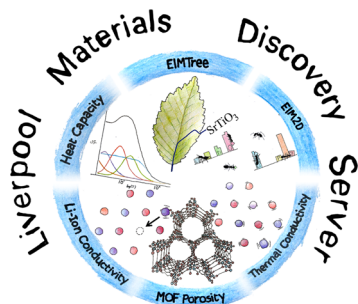
1589



Artificial intelligence aided recognition and classification of DNA nucleotides using MoS₂ nanochannels

Sneha Mittal, Souvik Manna, Milan Kumar Jena and Biswarup Pathak*

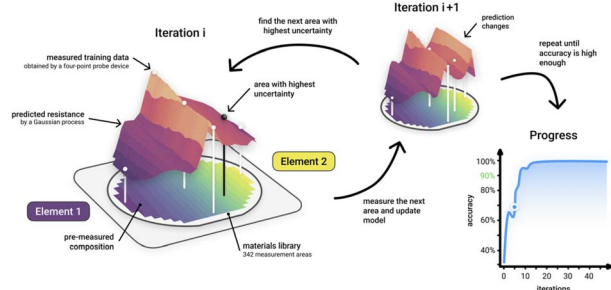
1601



The Liverpool materials discovery server: a suite of computational tools for the collaborative discovery of materials

Samantha Durdy, Cameron J. Hargreaves, Mark Dennison, Benjamin Wagg, Michael Moran, Jon A. Newnham, Michael W. Gaultois, Matthew J. Rosseinsky and Matthew S. Dyer*

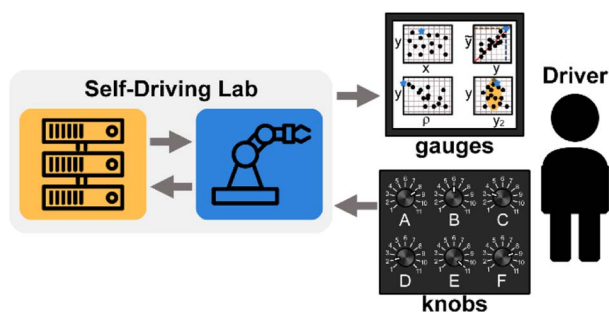
1612



Speeding up high-throughput characterization of materials libraries by active learning: autonomous electrical resistance measurements

Felix Thelen, Lars Banko, Rico Zehl, Sabrina Baha and Alfred Ludwig*

1620



Driving school for self-driving labs

Kelsey L. Snapp and Keith A. Brown*

