

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.

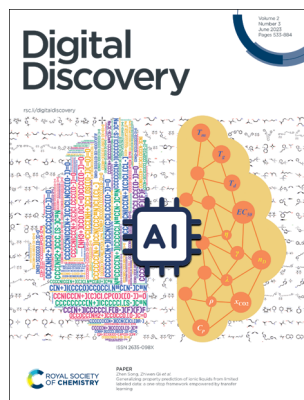
IN THIS ISSUE

ISSN 2635-098X CODEN DDIIAI 2(3) 533–884 (2023)



Cover

See Andy S. Anker, Keith T. Butler *et al.*, pp. 578–590. Image reproduced by permission of Andy S. Anker, Keith T. Butler, Manh Duc Le, Toby G. Perring and Jeyan Thiyagalingam from *Digital Discovery*, 2023, 2, 578. Created with the use of Midjourney.



Inside cover

See Zhen Song, Zhiwen Qi *et al.*, pp. 591–601. Image reproduced by permission of Guzhong Chen and Zhen Song from *Digital Discovery*, 2023, 2, 591.

PERSPECTIVES

544

The laboratory of Babel: highlighting community needs for integrated materials data management

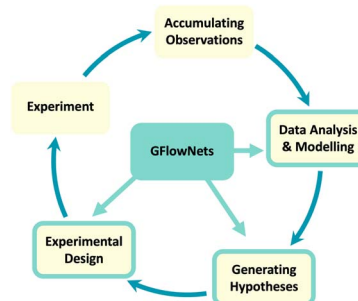
Brenden G. Pelkie and Lilo D. Pozzo*



557

GFlowNets for AI-driven scientific discovery

Moksh Jain,* Tristan Deleu, Jason Hartford, Cheng-Hao Liu, Alex Hernandez-Garcia and Yoshua Bengio



Editorial Staff

Editor

Anna Rulka

Deputy Editor

Audra Taylor

Editorial Production Manager

Viktoria Titmus

Assistant Editors

Shwetha Krishna, 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

Abigail Doyle, University of California Los Angeles, USA
Ola Engkvist, AstraZeneca and Chalmers University of Technology, Sweden
Pablo Carbonell, University of Valencia, Spain
Ian Foster, University of Chicago, USA
Cecilia Clementi, Freie Universität Berlin, Germany
Heather Kulik, MIT, USA

Silvana Botti, Friedrich Schiller University Jena, Germany
Marwin Segler, Microsoft, Germany
Jan Jensen, University of Copenhagen, Denmark
Berend Smit, EPFL, Switzerland
Conor Coley, MIT, USA
Koji Tsuda, The University of Tokyo, Japan
Isao Tanaka, Kyoto University, Japan

Shuye Ping Ong, University of California San Diego, USA
Alexandre Tkatchenko, University of Luxembourg, Luxembourg
Juan Alegre, Colorado State University, USA

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



Using generative adversarial networks to match experimental and simulated inelastic neutron scattering data

Generalizing property prediction of ionic liquids from limited labeled data: a one-stop framework empowered by transfer learning

Digital research environments: a requirements analysis

The diagram illustrates the PSDI Core architecture. At the center is the **PSDI Core**. Surrounding it is a ring of services: **Semantic Services**, **Domain based Databases**, **Domain based applications**, **P2P/LLNs**, **Equipment Interfaces**, **Literature Services**, **Automated decision**, and **Recommendation**. Outside this ring are several feature categories: **Collaboration & management**, **Other Features**, **Domain Features**, **Data Features**, **Notebooking Features**, **Generic Features**, and **Publishing & Sharing**. The background is decorated with colored ovals in shades of blue, purple, and orange.

Deep learning metal complex properties with natural quantum graphs

The diagram illustrates a workflow for predicting quantum material properties using Geometric and Electronic Information (GEO) and Graph Neural Networks (GNNs).

Input Data:

- Transition Metal Complexes:** Shown as a chemical structure of a transition metal complex (e.g., $\text{H}_2\text{C}=\text{CH}_2$ coordinated to a metal center).
- NBO Orbitals & SOPA Donor-Acceptor Interactions:** Shown as molecular orbitals and interaction diagrams (LP(d) to BD*(π^*)).

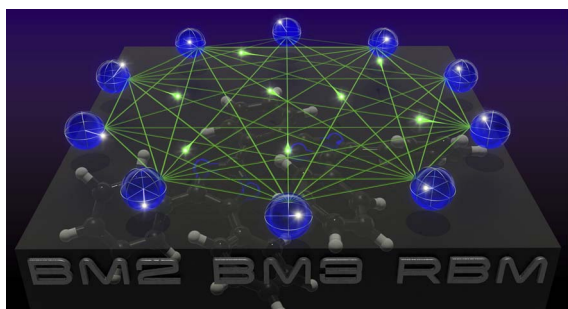
Processing:

- The input data is processed into **Natural Quantum Graphs (NatQG)**, which are categorized into *u-NatQG* (undirected) and *d-NatQG* (directed).
- The NatQG are then processed into the **tmQMg dataset**, which includes various material properties (e.g., E_{ZPE} , H , S , G , C_v , ϵ_0 , α , μ , V , \dots , CSV).

Output:

- The tmQMg dataset is used to train **GNNs Predicting Quantum Properties**, which are visualized as scatter plots of α vs ϵ .

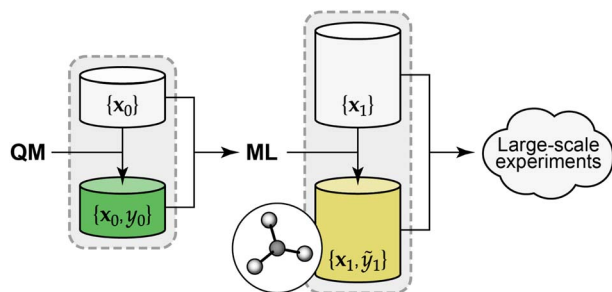
634



Artificial neural network encoding of molecular wavefunctions for quantum computing

Masaya Hagai,^{*} Mahito Sugiyama, Koji Tsuda and Takeshi Yanai^{*}

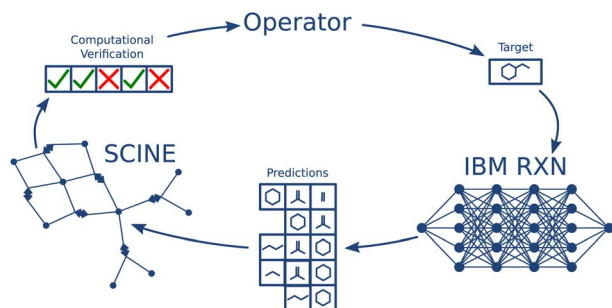
651



Synthetic data enable experiments in atomistic machine learning

John L. A. Gardner, Zoé Faure Beaulieu and Volker L. Deringer^{*}

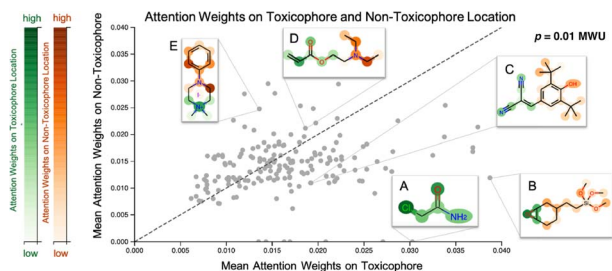
663



Quantum chemical data generation as fill-in for reliability enhancement of machine-learning reaction and retrosynthesis planning

Alessandra Toniato, Jan P. Unsleber, Alain C. Vaucher, Thomas Weymuth, Daniel Probst, Teodoro Laino^{*} and Markus Reiher^{*}

674



Chemical representation learning for toxicity prediction

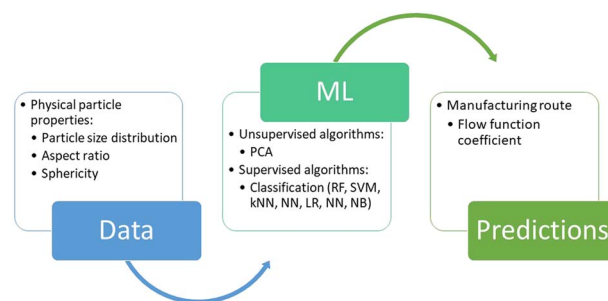
Jannis Born,^{*} Greta Markert, Nikita Janakaraman, Talia B. Kimber, Andrea Volkamer, María Rodríguez Martínez and Matteo Manica



692

Machine learning approaches to the prediction of powder flow behaviour of pharmaceutical materials from physical properties

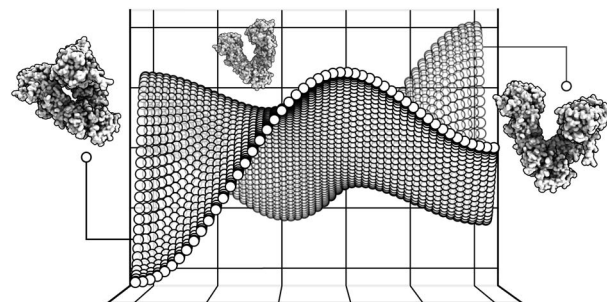
Laura Pereira Diaz, Cameron J. Brown, Ebenezer Ojo, Chantal Mustoe and Alastair J. Florence*



702

Beyond ManifoldEM: geometric relationships between manifold embeddings of a continuum of 3D molecular structures and their 2D projections

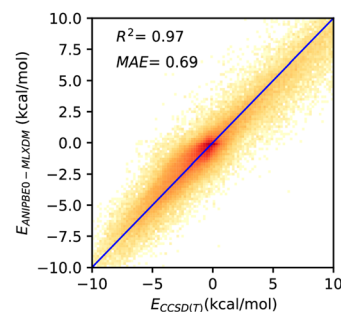
Evan Seitz, Joachim Frank* and Peter Schwander*



718

A neural network potential with rigorous treatment of long-range dispersion

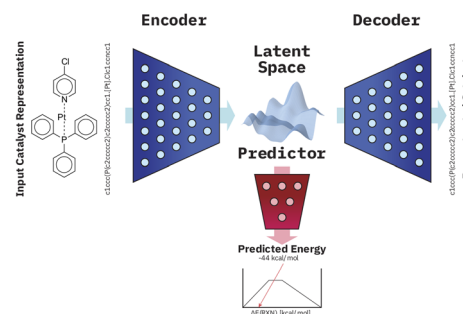
Nguyen Thien Phuc Tu,* Nazanin Rezajooei, Erin R. Johnson* and Christopher N. Rowley*

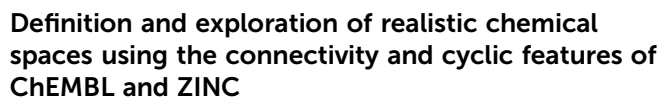


728

Designing catalysts with deep generative models and computational data. A case study for Suzuki cross coupling reactions

Oliver Schilter,* Alain Vaucher, Philippe Schwaller and Teodoro Laino





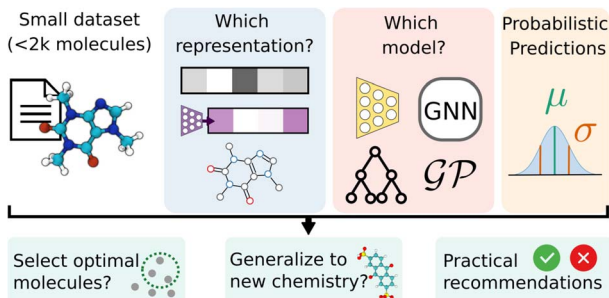
Thomas Cauchy,* Jules Leguy and Benoit Da Mota*

748



Austin H. Cheng,* Andy Cai, Santiago Miret,
Gustavo Malkomes, Mariano Phielipp and
Alán Aspuru-Guzik

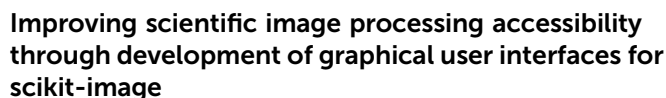
759



Calibration and generalizability of probabilistic models on low-data chemical datasets with DIONYSUS

Gary Tom, Riley J. Hickman, Aniket Zinzuwadia,
Afshan Mohajeri, Benjamin Sanchez-Lengeling
and Alán Aspuru-Guzik*

775



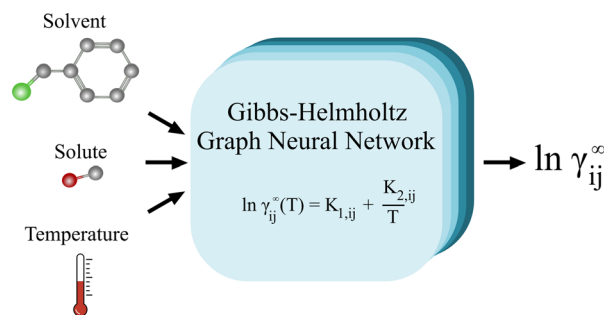
Mikael Kuwahara, Jun Fujima, Keisuke Takahashi*
and Lauren Takahashi*

PAPERS

781

Gibbs–Helmholtz graph neural network: capturing the temperature dependency of activity coefficients at infinite dilution

Edgar Ivan Sanchez Medina, Steffen Linke, Martin Stoll and Kai Sundmacher*



799

Automated electrolyte formulation and coin cell assembly for high-throughput lithium-ion battery research

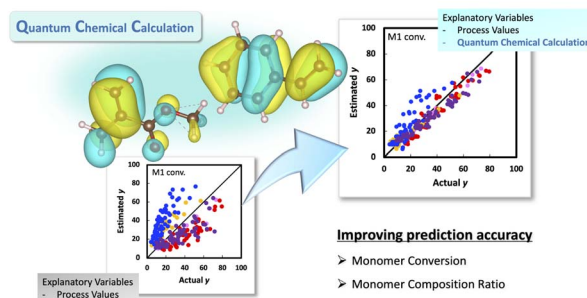
Jackie T. Yik,* Leiting Zhang,* Jens Sjölund, Xu Hou, Per H. Svensson, Kristina Edström and Erik J. Berg



809

Extrapolation performance improvement by quantum chemical calculations for machine-learning-based predictions of flow-synthesized binary copolymers

Shogo Takasuka, Shunto Oikawa, Takayoshi Yoshimura, Sho Ito, Yosuke Harashima, Tomoaki Takayama, Shigehito Asano, Akira Kurosawa, Tetsunori Sugawara, Miho Hatanaka, Tomoyuki Miyao, Takamitsu Matsubara, Yu-ya Ohnishi, Hiroharu Ajiro and Mikiya Fujii*



819

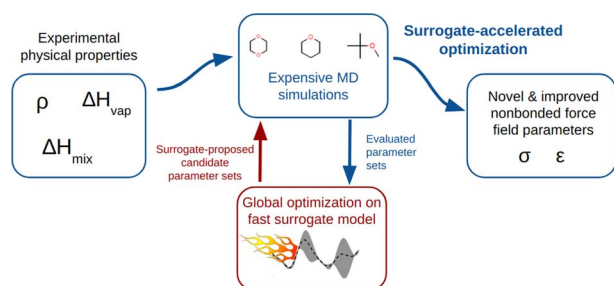
Predicting ruthenium catalysed hydrogenation of esters using machine learning

Challenger Mishra,* Niklas von Wolff,* Abhinav Tripathi, Claire N. Brodie, Neil D. Lawrence, Aditya Ravuri, Éric Brémond, Annika Preiss and Amit Kumar*



PAPERS

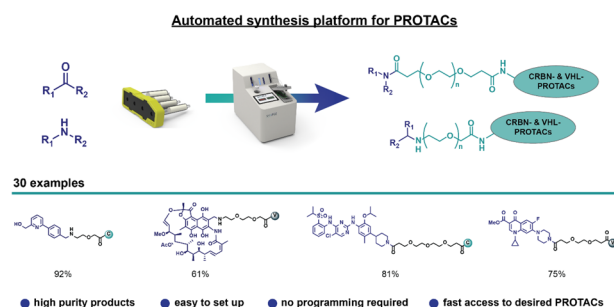
828



Using physical property surrogate models to perform accelerated multi-fidelity optimization of force field parameters

Owen C. Madin and Michael R. Shirts*

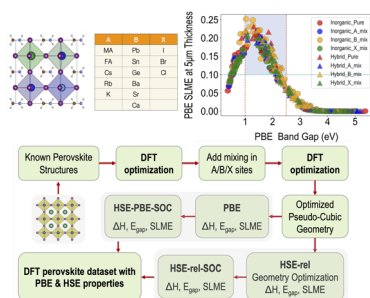
848



Capsule-based automated synthesis for the efficient assembly of PROTAC like molecules

Samuele Bordi, Tuo Jiang, Anna Konopka, Guillaume Coin, Paula L. Nichols and Benedikt M. Wanner*

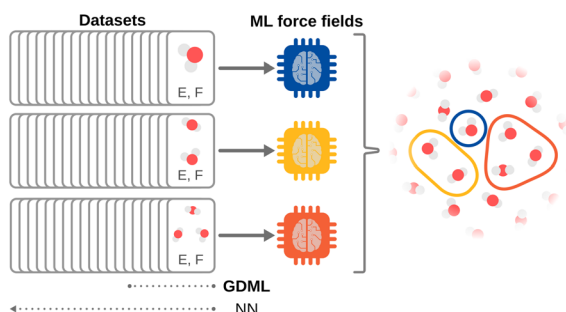
856



A high-throughput computational dataset of halide perovskite alloys

Jiaqi Yang, Panayotis Manganaris and Arun Mannodi-Kanakthodi*

871



Modeling molecular ensembles with gradient-domain machine learning force fields

Alex M. Maldonado, Igor Poltavsky, Valentin Vassilev-Galindo, Alexandre Tkatchenko* and John A. Keith*



CORRECTIONS

881

Correction: Molecular sonification for molecule to music information transfer

Babak Mahjour, Jordan Bench, Rui Zhang, Jared Frazier and Tim Cernak*

882

Correction: Latent spaces for antimicrobial peptide design

Samuel Renaud and Rachael A. Mansbach*

