

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(2) 251–532 (2023)



Cover

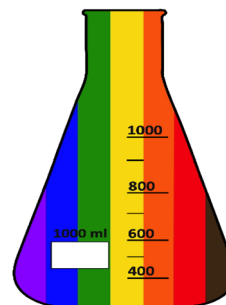
See Isaac Squires *et al.*, pp. 316–326. Image reproduced by permission of Isaac Squires and Keion Ing, *Digital Discovery*, 2023, 2, 316.

OPINION

260

Academic free speech or right-wing grievance?

John M. Herbert*

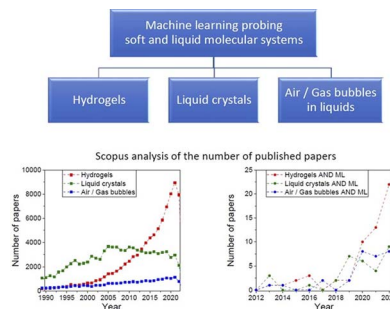


REVIEW

298

Machine learning for soft and liquid molecular materials

Tetiana Orlova, Anastasiia Piven, Darina Darmoroz, Timur Aliev, Tamer Mahmoud Tamer Abdel Razik, Anton Boitsev, Natalia Grafeeva and Ekaterina Skorb*



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.

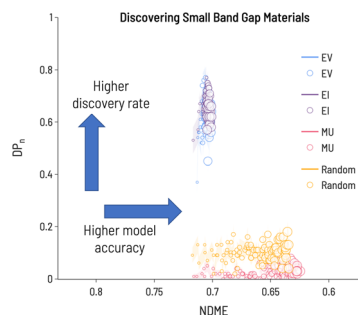
Registered charity number: 207890



Isaac Squires,* Amir Dahari, Samuel J. Cooper
and Steve Kench

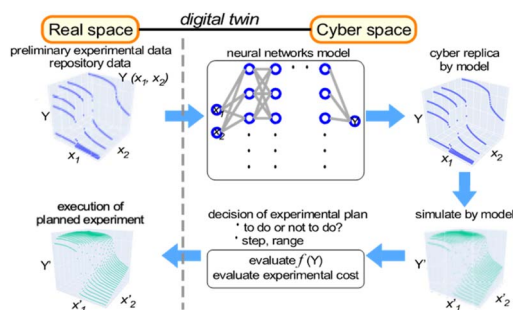
327

Christopher K. H. Borg,^{*} Eric S. Muckley, Clara Nyby,
James E. Saal, Logan Ward, Apurva Mehta
and Bryce Meredig



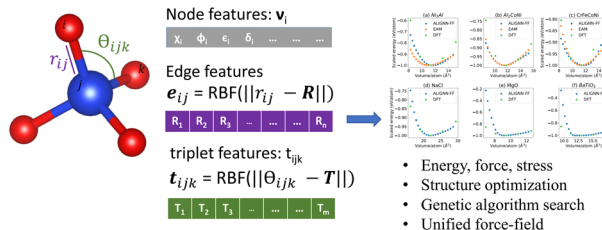
339

Kensei Terashima,* Pedro Baptista de Castro, Miren Garbiñe Esparza Echevarria, Ryo Matsumoto, Takafumi D. Yamamoto, Akiko T. Saito, Hiroyuki Takeya and Yoshihiko Takano



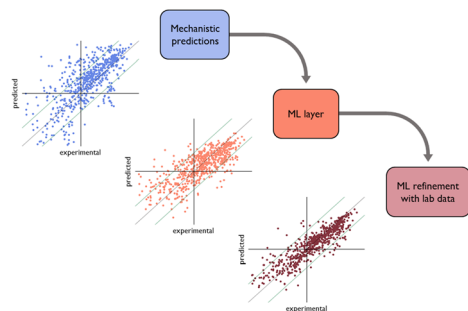
346

Kamal Choudhary,* Brian DeCost, Lily Major, Keith Butler,
Jeyan Thiyaqalingam and Francesca Tavazza



PAPERS

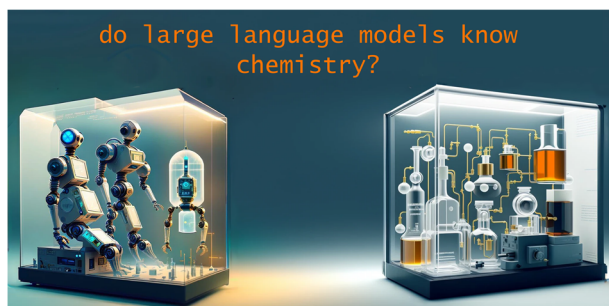
356



A unified ML framework for solubility prediction across organic solvents

Antony D. Vassileiou,^{*} Murray N. Robertson, Bruce G. Wareham, Mithushan Soundaranathan, Sara Ottoboni, Alastair J. Florence, Thoralf Hartwig and Blair F. Johnston^{*}

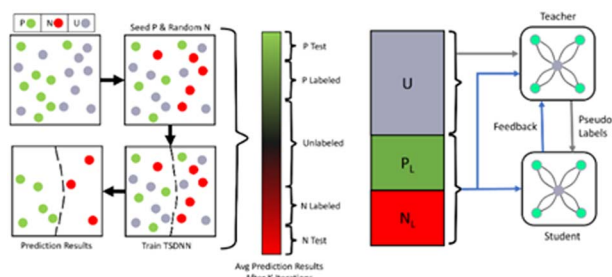
368



Assessment of chemistry knowledge in large language models that generate code

Andrew D. White,^{*} Glen M. Hocky,^{*} Heta A. Gandhi, Mehrad Ansari, Sam Cox, Geemi P. Wellawatte, Subarna Sasmal, Ziyue Yang, Kangxin Liu, Yuvraj Singh and Willmor J. Peña Ccoa

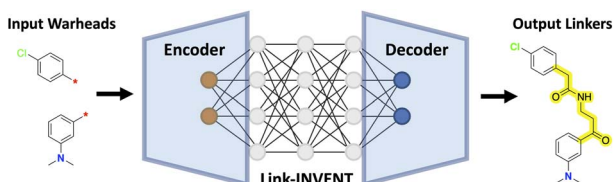
377



Materials synthesizability and stability prediction using a semi-supervised teacher-student dual neural network

Daniel Gleaves, Nihang Fu, Edirisuriya M. Dilanga Siriwardane, Yong Zhao and Jianjun Hu^{*}

392



Link-INVENT: generative linker design with reinforcement learning

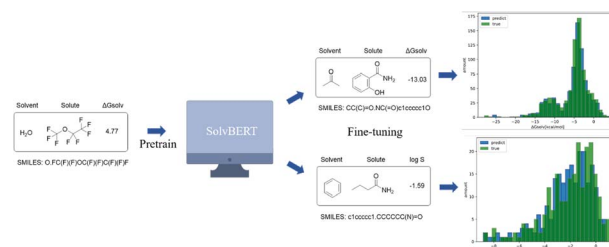
Jeff Guo, Franziska Knuth, Christian Margreitter, Jon Paul Janet, Kostas Papadopoulos, Ola Engkvist and Atanas Patronov^{*}



409

SolvBERT for solvation free energy and solubility prediction: a demonstration of an NLP model for predicting the properties of molecular complexes

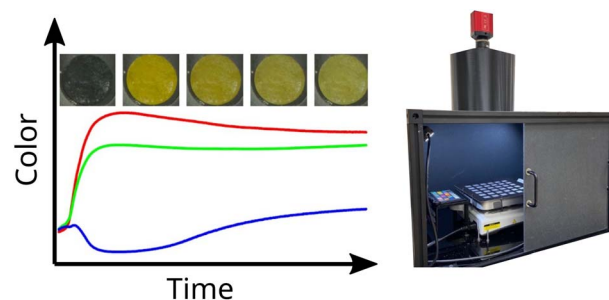
Jiahui Yu, Chengwei Zhang, Yingying Cheng, Yun-Fang Yang, Yuan-Bin She, Fengfan Liu, Weike Su and An Su*



422

An open-source environmental chamber for materials-stability testing using an optical proxy

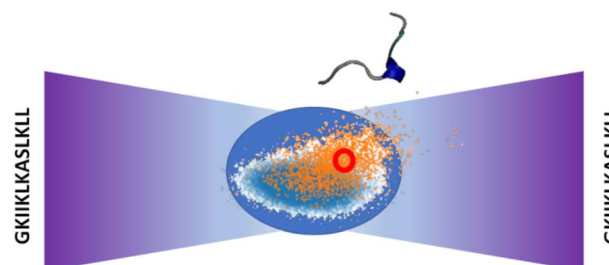
Rodolfo Keesey,* Armi Tiihonen,* Alexander E. Siemenn, Thomas W. Colburn, Shijing Sun, Noor Titan Putri Hartono, James Serdy, Margaret Zeile, Keqing He, Cole A. Gurtner, Austin C. Flick, Clio Batali, Alex Encinas, Richa R. Naik, Zhe Liu, Felipe Oviedo, I. Marius Peters, Janak Thapa, Siyu Isaac Parker Tian, Reinhold H. Dauskardt, Alexander J. Norquist* and Tonio Buonassisi*



441

Latent spaces for antimicrobial peptide design

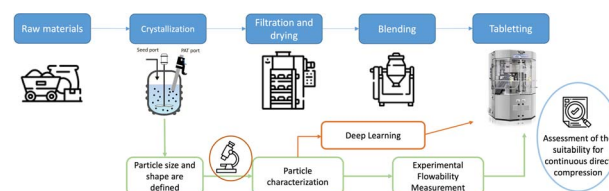
Samuel Renaud and Rachael A. Mansbach*



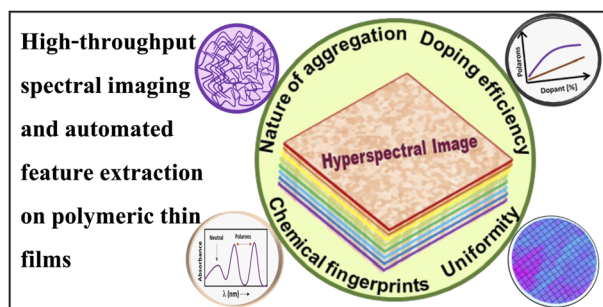
459

Predicting pharmaceutical powder flow from microscopy images using deep learning

Matthew R. Wilkinson,* Laura Pereira Diaz, Antony D. Vassileiou, John A. Armstrong, Cameron J. Brown, Bernardo Castro-Dominguez and Alastair J. Florence*



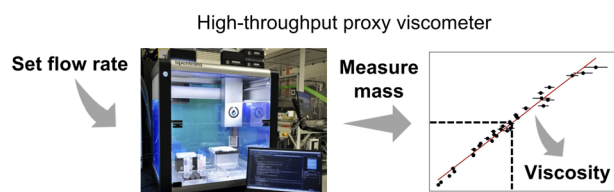
471



Diagnosis of doped conjugated polymer films using hyperspectral imaging

Vijila Chellappan,* Adithya Kumar, Saif Ali Khan, Pawan Kumar and Kedar Hippalgaonkar*

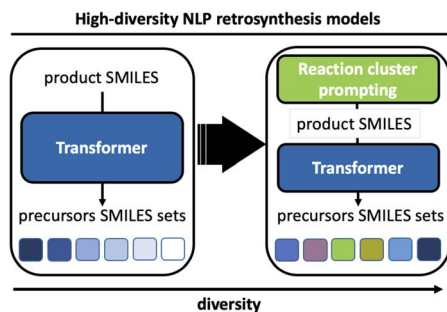
481



Automated pipetting robot for proxy high-throughput viscometry of Newtonian fluids

Beatrice W. Soh, Aniket Chitre, Wen Yang Lee, Daniil Bash, Jatin N. Kumar and Kedar Hippalgaonkar*

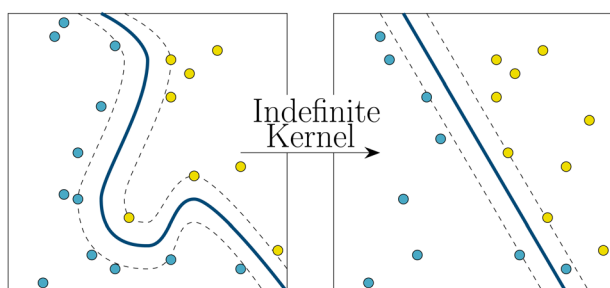
489



Enhancing diversity in language based models for single-step retrosynthesis

Alessandra Toniato,* Alain C. Vaucher, Philippe Schwaller and Teodoro Laino

502



Krein support vector machine classification of antimicrobial peptides

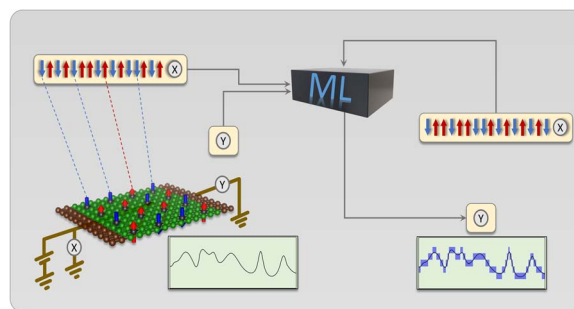
Joseph Redshaw, Darren S. J. Ting, Alex Brown, Jonathan D. Hirst* and Thomas Gärtner



512

Classical and quantum machine learning applications in spintronics

Kumar J. B. Ghosh* and Sumit Ghosh*



520

Molecular sonification for molecule to music information transfer

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

