

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(4) 885–1220 (2023)



Cover

See Safa Jamali *et al.*, pp. 915–928. Image reproduced by permission of Safa Jamali and Milad Saadat from *Digital Discovery*, 2023, 2, 915.



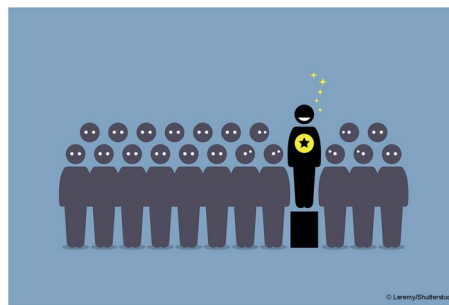
Inside cover

See María Victoria Gil, Berend Smit *et al.*, pp. 929–940. Image reproduced by permission of María Victoria Gil Matellanes from *Digital Discovery*, 2023, 2, 929. This image was created by Kevin Jablonka using Midjourney.

EDITORIAL

896

Outstanding Reviewers for *Digital Discovery* in 2022



TUTORIAL REVIEW

897

Recent advances in the self-referencing embedded strings (SELFIES) library

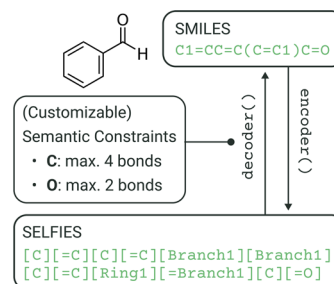
Alston Lo,* Robert Pollice, AkshatKumar Nigam, Andrew D. White, Mario Krenn and Alán Aspuru-Guzik

selfies

2022: v2.1.1

- More molecules supported
- Added customizability
- Streamlined and generalized grammar
- Cleaner and faster code
- QoL improvements

2019: v0.2.4



Editorial Staff

Editor

Anna Rulka

Deputy Editor

Audra Taylor

Editorial Production Manager

Viktoria Titmus

Assistant Editors

Angelica-Jane Kechinyere Onyekwere, 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 com-
putation 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

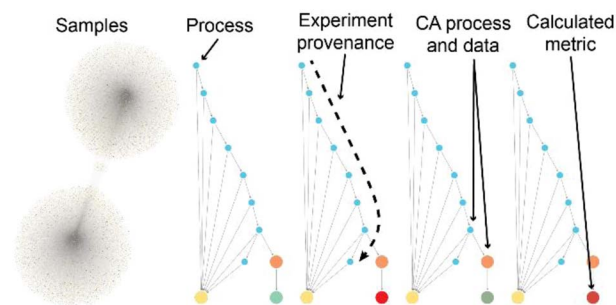


COMMUNICATION

909

The materials experiment knowledge graph

Michael J. Statt,* Brian A. Rohr,* Dan Guevarra,
Ja'Nya Breeden, Santosh K. Suram and John M. Gregoire*

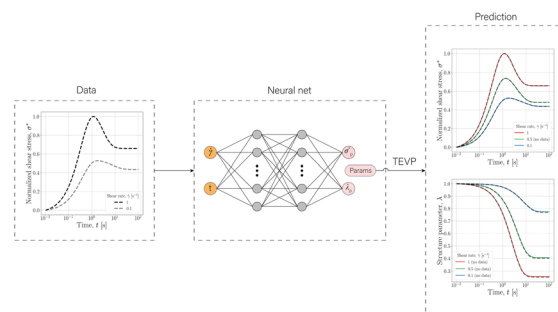


PAPERS

915

A rheologist's guideline to data-driven recovery of complex fluids' parameters from constitutive models

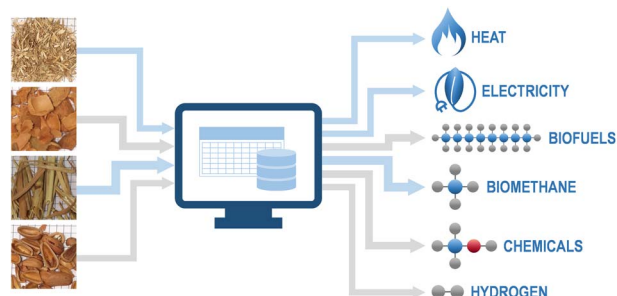
Milad Saadat, Deepak Mangal and Safa Jamali*



929

Biomass to energy: a machine learning model for optimum gasification pathways

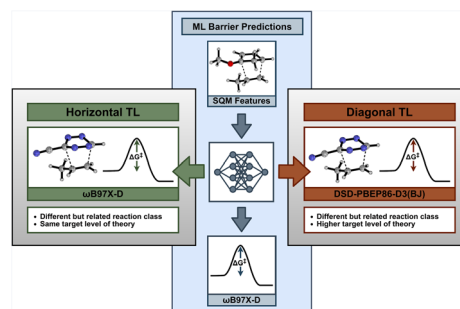
María Victoria Gil,* Kevin Maik Jablonka, Susana Garcia,
Covadonga Pevida and Berend Smit*



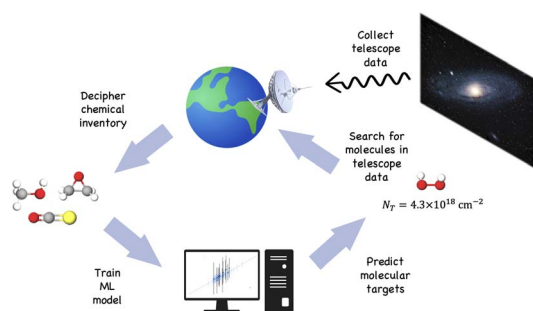
941

Machine learning reaction barriers in low data regimes: a horizontal and diagonal transfer learning approach

Samuel G. Espley, Elliot H. E. Farrar, David Buttar,
Simone Tomasi and Matthew N. Grayson*



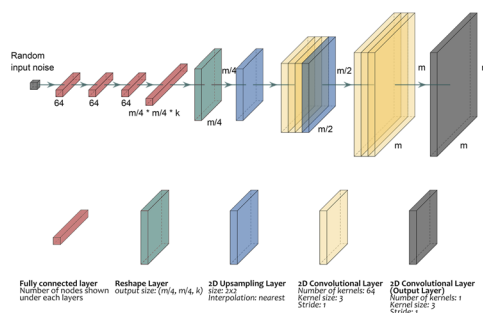
952



Implementation of rare isotopologues into machine learning of the chemical inventory of the solar-type protostellar source IRAS 16293-2422

Zachary T. P. Fried,^{*} Kin Long Kelvin Lee, Alex N. Byrne and Brett A. McGuire^{*}

967

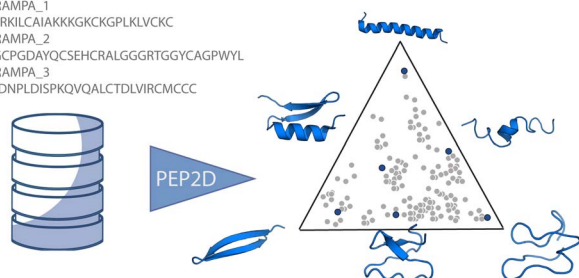


A scalable neural network architecture for self-supervised tomographic image reconstruction

Hongyang Dong, Simon D. M. Jacques, Winfried Kockelmann, Stephen W. T. Price, Robert Emberson, Dorota Matras, Yaroslav Odarchenko, Vesna Middelkoop, Athanasios Giokaris, Olof Gutowski, Ann-Christin Dippel, Martin von Zimmermann, Andrew M. Beale, Keith T. Butler^{*} and Antonis Vamvakeros^{*}

981

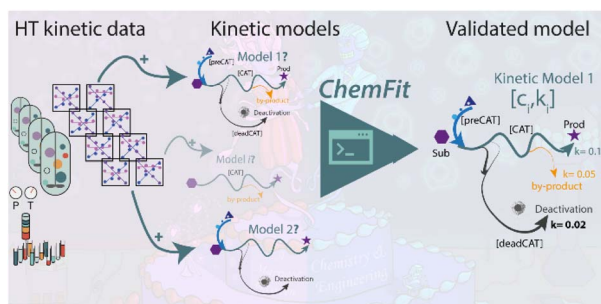
>GRAMPA_1
GLPRKILCAIAKKKGKCKGPKLVCKC
>GRAMPA_2
GFGCPGDAYQCSEHCRA LGGGRTGGYAGPWYL
>GRAMPA_3
LVKDNPLDISPKQVQALCTDLVIRCMCCC
...



Benchmarking protein structure predictors to assist machine learning-guided peptide discovery

Victor Daniel Aldas-Bulos and Fabien Plisson^{*}

994



Model-based evaluation and data requirements for parallel kinetic experimentation and data-driven reaction identification and optimization

Nathan Jiscot, Evgeny A. Uslamin^{*} and Evgeny A. Pidko^{*}

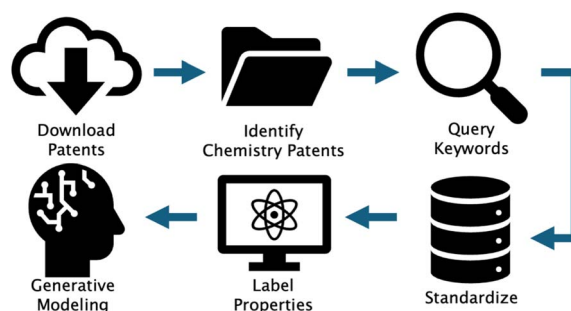


PAPERS

1006

Automated patent extraction powers generative modeling in focused chemical spaces

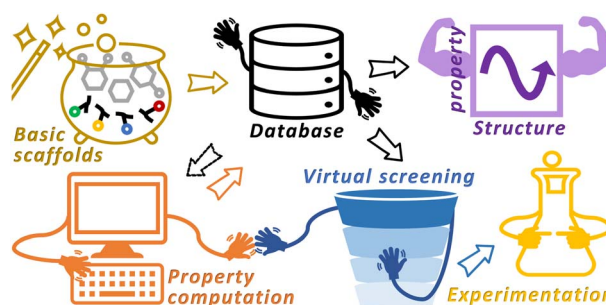
Akshay Subramanian, Kevin P. Greenman, Alexis Gervais, Tzuhsiung Yang and Rafael Gómez-Bombarelli*



1016

Discovery of lead quinone cathode materials for Li-ion batteries

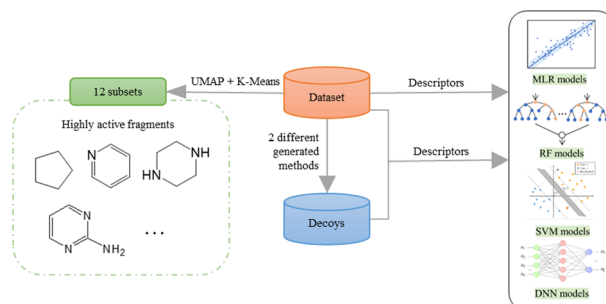
Xuan Zhou, Abhishek Khetan, Jie Zheng, Mark Huijben, René A. J. Janssen and Süleyman Er*



1026

A SAR and QSAR study on cyclin dependent kinase 4 inhibitors using machine learning methods

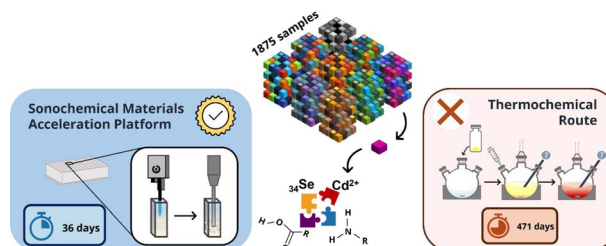
Xiaoyang Pang, Yuniang Zhao, Guo Li, Jianrong Liu* and Aixia Yan*



1042

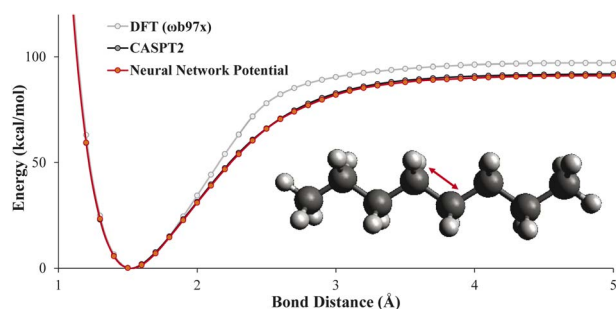
A high-throughput workflow for the synthesis of CdSe nanocrystals using a sonochemical materials acceleration platform

Maria Politi, Fabio Baum, Kiran Vaddi, Edwin Antonio, Joshua Vasquez, Brittany P. Bishop, Nadya Peek, Vincent C. Holmberg and Lilo D. Pozzo*



PAPERS

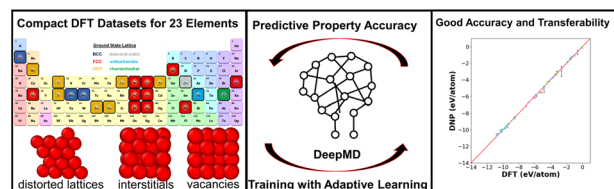
1058



Neural network potentials for reactive chemistry: CASPT2 quality potential energy surfaces for bond breaking

Quin H. Hu, Andrew M. Johannesen, Daniel S. Graham and Jason D. Goodpaster*

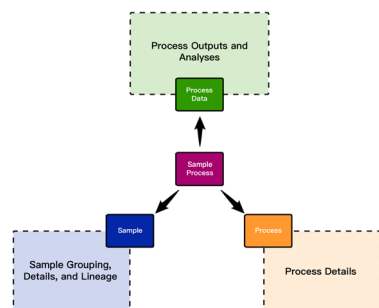
1070



Highly transferable atomistic machine-learning potentials from curated and compact datasets across the periodic table

Christopher M. Andolina and Wissam A. Saidi*

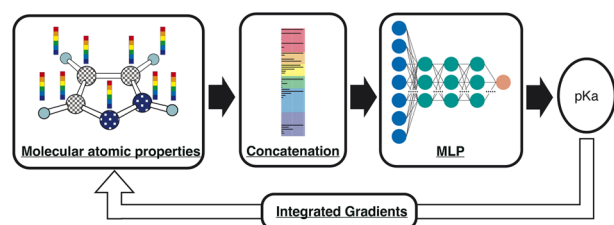
1078



ESAMP: event-sourced architecture for materials provenance management and application to accelerated materials discovery

Michael J. Statt,* Brian A. Rohr, Kris Brown, Dan Guevarra, Jens Hummelshøj, Linda Hung, Abraham Anapolsky, John M. Gregoire* and Santosh K. Suram*

1089



Accuracy & Overcorrelation & Interpretability

Feature selection in molecular graph neural networks based on quantum chemical approaches

Daisuke Yokogawa* and Kayo Suda

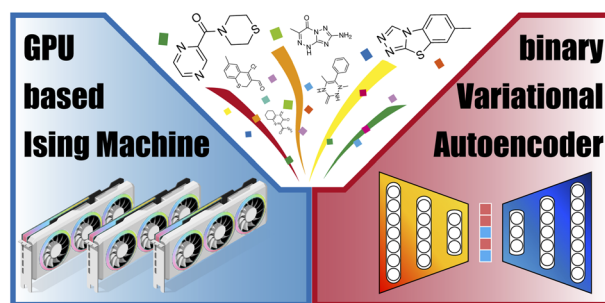


PAPERS

1098

Chemical design with GPU-based Ising machines

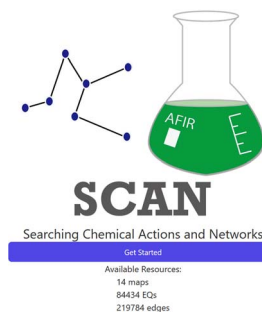
Zetian Mao, Yoshiki Matsuda, Ryo Tamura* and Koji Tsuda*



1104

Searching chemical action and network (SCAN): an interactive chemical reaction path network platform

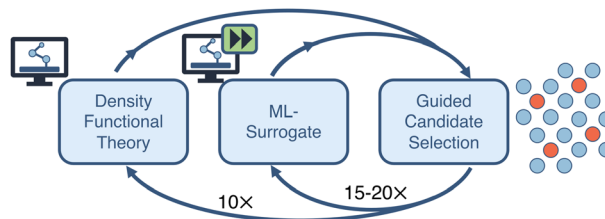
Mikael Kuwahara, Yu Harabuchi, Satoshi Maeda,* Jun Fujima* and Keisuke Takahashi*



1112

By how much can closed-loop frameworks accelerate computational materials discovery?

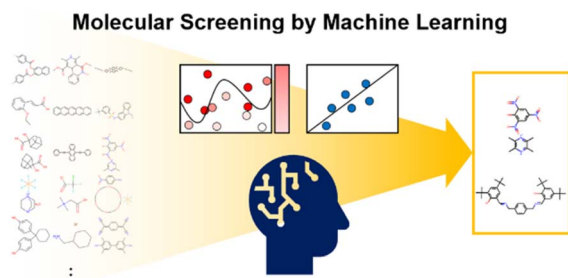
Lance Kavalsky, Vinay I. Hegde, Eric Muckley, Matthew S. Johnson, Bryce Meredig* and Venkatasubramanian Viswanathan*



1126

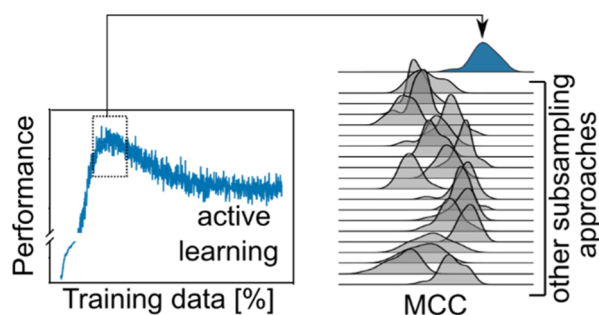
Molecular screening for solid–solid phase transitions by machine learning

Daisuke Takagi, Kazuki Ishizaki, Toru Asahi and Takuya Taniguchi*



PAPERS

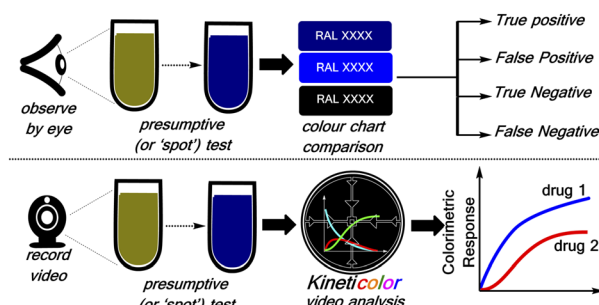
1134



Improving molecular machine learning through adaptive subsampling with active learning

Yujing Wen, Zhixiong Li, Yan Xiang and Daniel Reker*

1143



Teaching old presumptive tests new digital tricks with computer vision for forensic applications

Nathalie Bugeja, Cameron Oliver, Nicole McGrath, Jake McGuire, Chunhui Yan, Felicity Carlisle-Davies and Marc Reid*

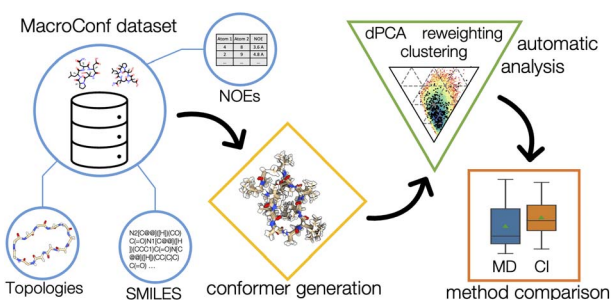
1152



Towards a comprehensive data infrastructure for redox-active organic molecules targeting non-aqueous redox flow batteries

Rebekah Duke, Vinayak Bhat, Parker Sornberger, Susan A. Odom and Chad Risko*

1163



MacroConf – dataset & workflows to assess cyclic peptide solution structures

Daniel Crusius, Jason R. Schnell, Flaviu Cipcigan and Philip C. Biggin*

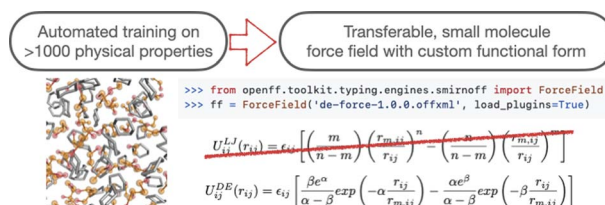


PAPERS

1178

A transferable double exponential potential for condensed phase simulations of small molecules

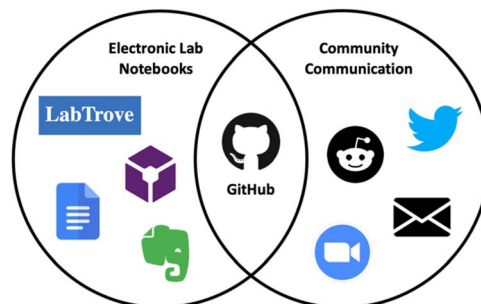
Joshua T. Horton, Simon Boothroyd,
Pavan Kumar Behara, David L. Mobley and Daniel J. Cole*



1188

GitHub as an open electronic laboratory notebook for real-time sharing of knowledge and collaboration

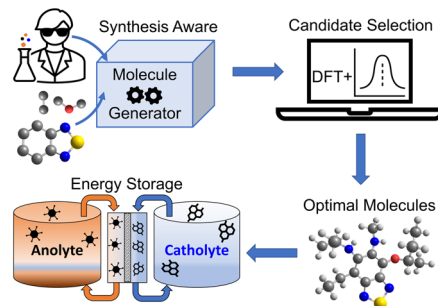
Kymberley R. Scroggie, Klementine J. Burrell-Sander,
Peter J. Rutledge and Alice Motion*



1197

In silico discovery of a new class of anolyte redoxmers for non-aqueous redox flow batteries

Akash Jain, Ilya A. Shkrob, Hieu A. Doan, Lily A. Robertson,
Lu Zhang and Rajeev S. Assary*



1209

A scientific machine learning framework to understand flash graphene synthesis

Kianoosh Sattari, Lucas Eddy, Jacob L. Beckham,
Kevin M. Wyss, Richard Byfield, Long Qian,
James M. Tour* and Jian Lin*

