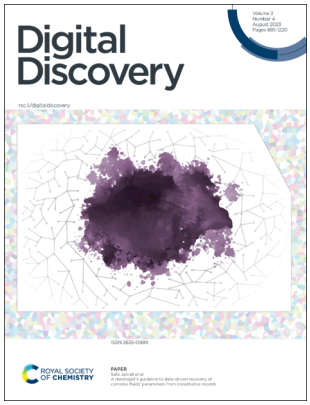
Digital Discovery

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

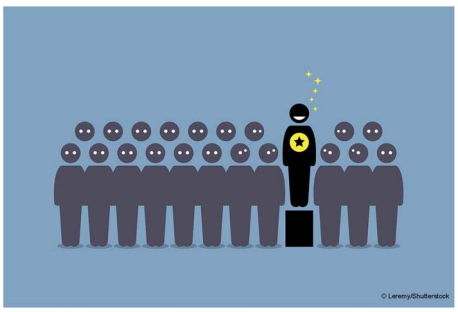
ISSN 2635-098X CODEN DDIIAI 2(4) 885–1220 (2023)



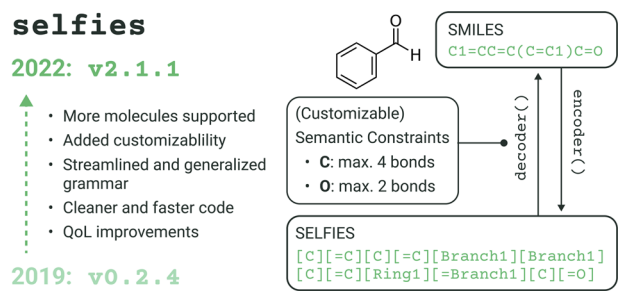
Cover
See Safa Jamali *et al.*, pp. 915–928. Image reproduced by permission of Safa Jamali and Milad Saadat from *Digital Discovery*, 2023, **2**, 915.

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



TUTORIAL REVIEW



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

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.

Information for Authors

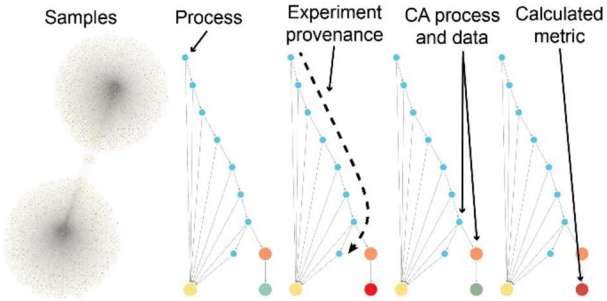
Full details on how to submit material for publication in Digital Discovery are given in the Instructions for Authors (available from http://www.rsc.org/authors). Submissions should be made via the journal's homepage: rsc.li/digitaldiscovery

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.

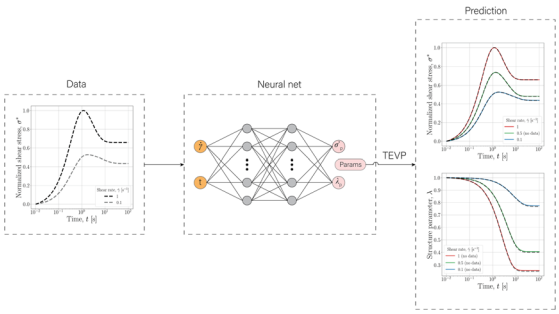
Registered charity number: 207890

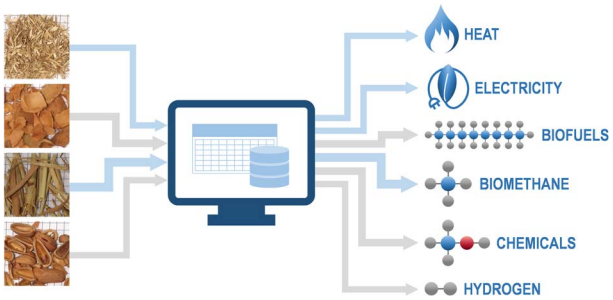
ROYAL SOCIETY OF CHEMISTRY

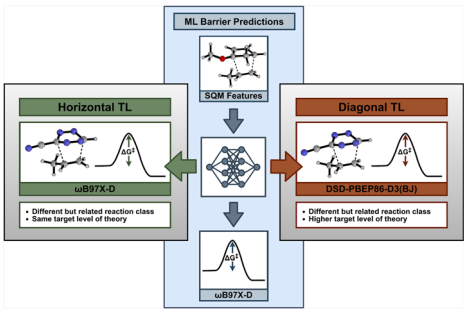
COMMUNICATION



PAPERS

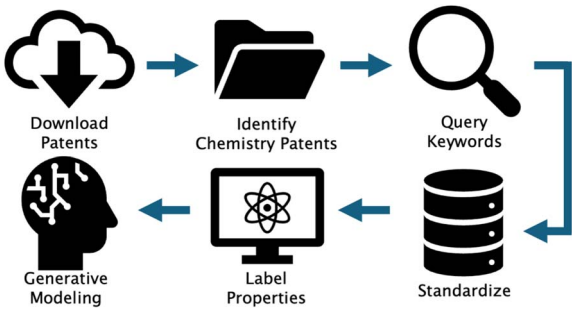


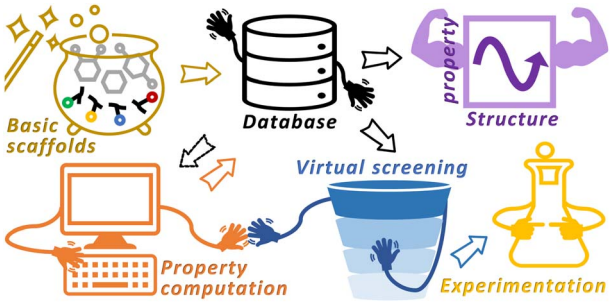


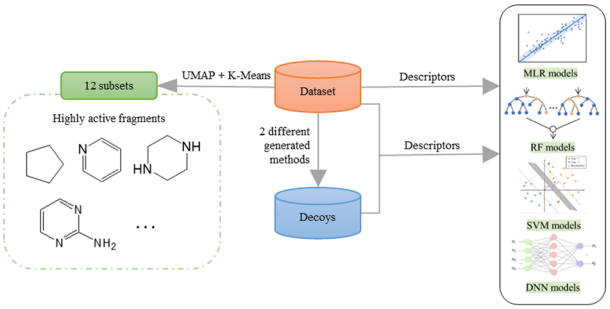


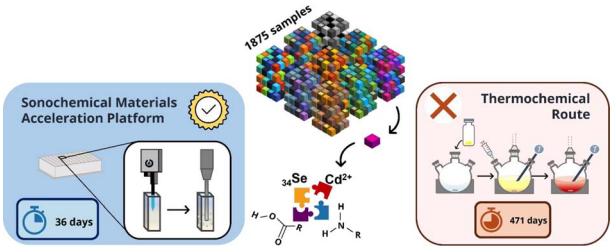
PAPERS

PAPERS



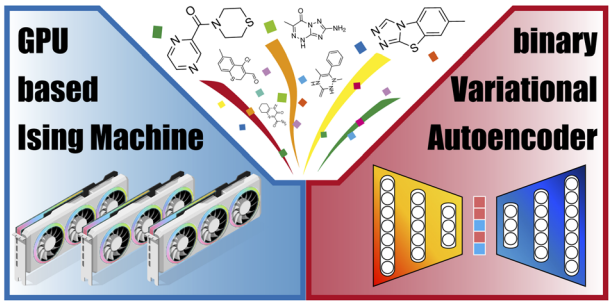


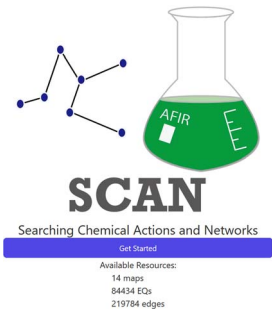


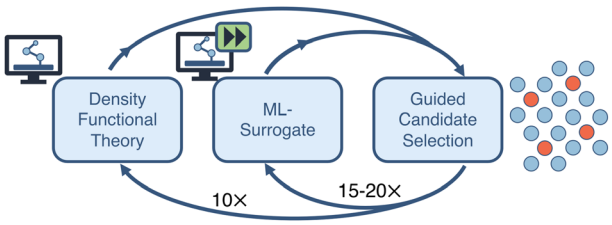


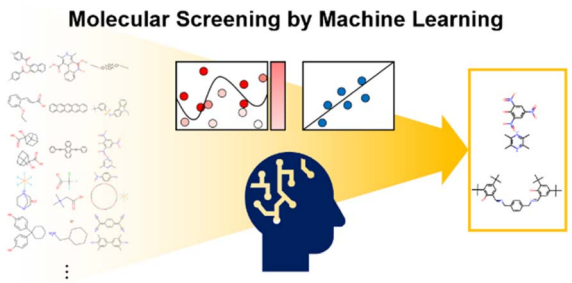
PAPERS

PAPERS









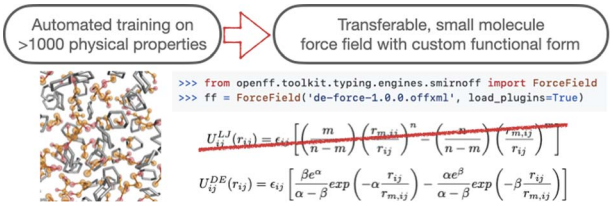
PAPERS

PAPERS

1178

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

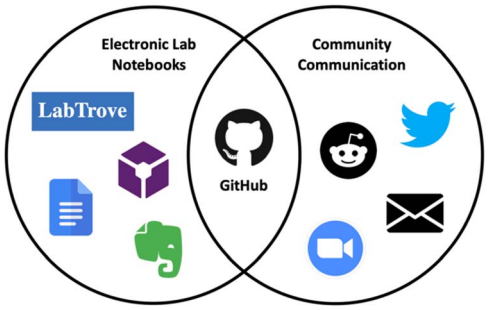
Joshua T. Horton, Simon Boothroyd, Pavan Kumar Behara, David L. Mobley and Daniel J. Cole*



1188

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

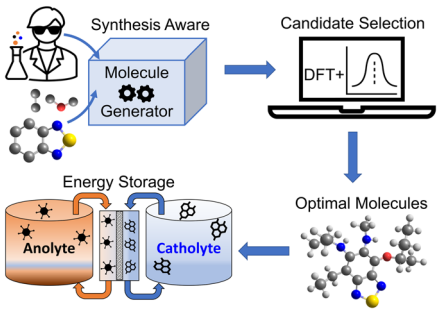
Kymberley R. Scroggie, Klementine J. Burrell-Sander, Peter J. Rutledge and Alice Motion*



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*