

# Digital Discovery

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ISSN 2635-098X CODEN DDIIAI 5(1) 1–466 (2026)



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See Keith A. Brown *et al.*, pp. 14–27. Image reproduced by permission of Adedire D. Adesiji from *Digital Discovery*, 2026, 5, 14.



### Inside cover

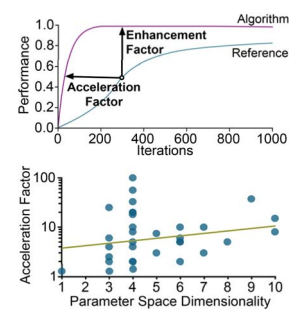
See Connor Forster and Carolin Müller, pp. 98–107. Image reproduced by permission of C. Forster and C. Müller from *Digital Discovery*, 2026, 5, 98.

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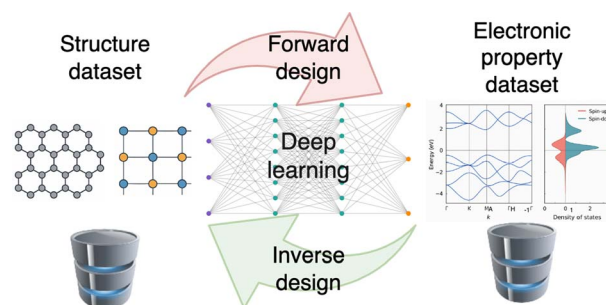
Adedire D. Adesiji, Jiashuo Wang, Cheng-Shu Kuo and Keith A. Brown\*



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Artem Mishchenko,\* Anupam Bhattacharya,\* Xiangwen Wang, Henry Kelbrick Pentz, Yihao Wei and Qian Yang



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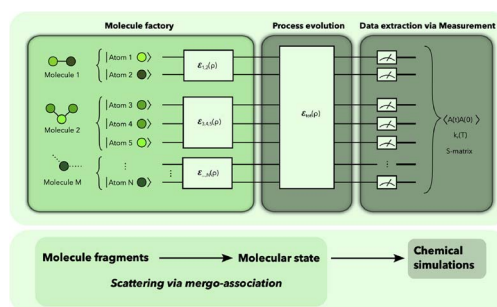


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## Chemically motivated simulation problems are efficiently solvable on a quantum computer

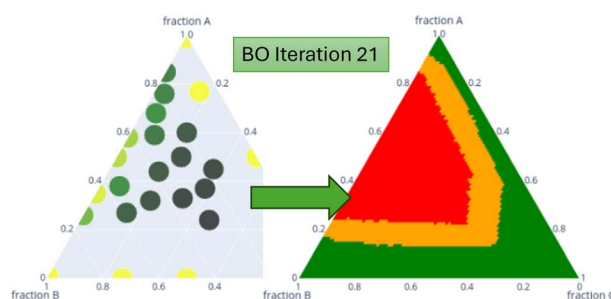
Philipp Schleich,\* Lasse Bjørn Kristensen, Jorge A. Campos-Gonzalez-Angulo, Abdulrahman Aldossary, Davide Avagliano, Mohsen Bagherimehrab, Christoph Gorgulla, Joe Fitzsimons and Alán Aspuru-Guzik



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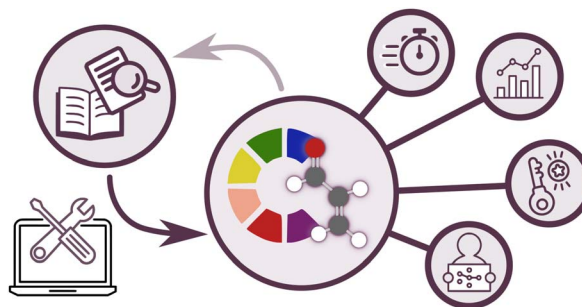
Naruki Yoshikawa,\* Kevin Angers, Kourosh Darvish, Sargol Okhovatian, Dawn Bannerman, Ilya Yakavets, Milica Radisic\* and Alán Aspuru-Guzik\*



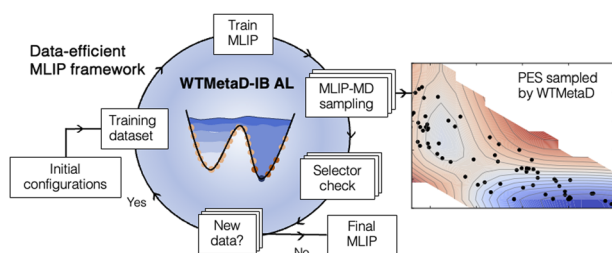
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## From handbooks to high-throughput: rule-based prediction of electronic absorption maxima from SMILES with ChromoPredict

Connor Forster and Carolin Müller\*



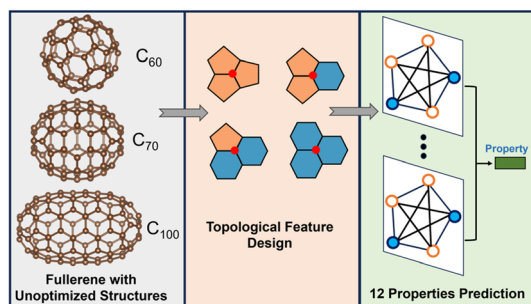
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Valdas Vitartas, Hanwen Zhang, Veronika Juraskova, Tristan Johnston-Wood and Fernanda Duarte\*

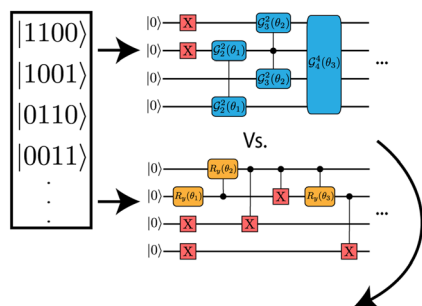
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Bin Liu, Jirui Jin and Mingjie Liu\*

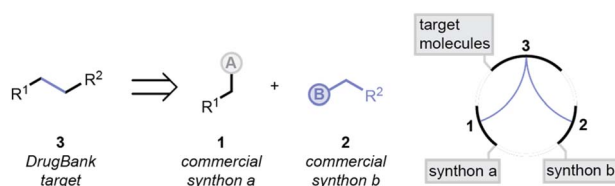
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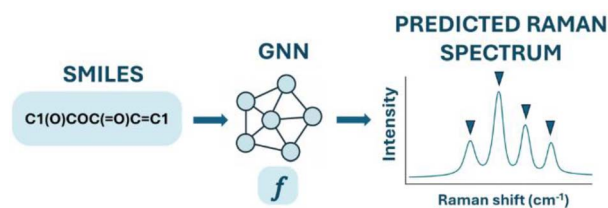
Babak Mahjour, Felix Katzenburg, Emil Lammi and Tim Cernak\*



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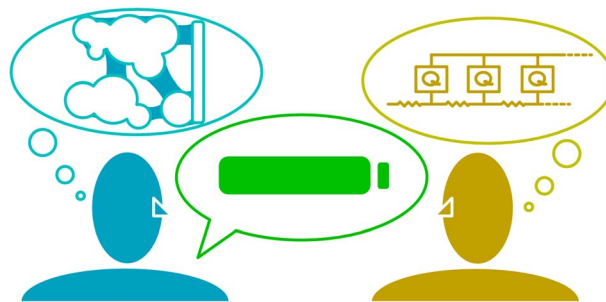
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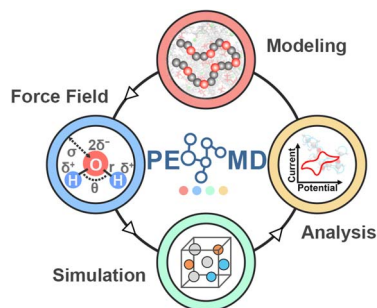
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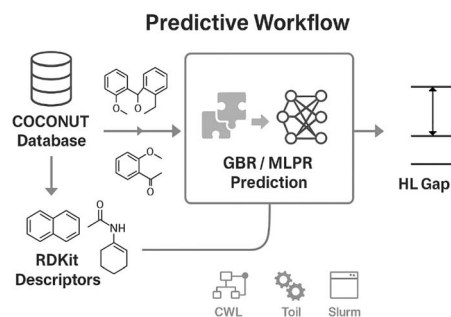
Shendong Tan, Bochun Liang, Dexin Lu, Chaoyuan Ji, Wenke Ji, Zihui Li and Tingzheng Hou\*



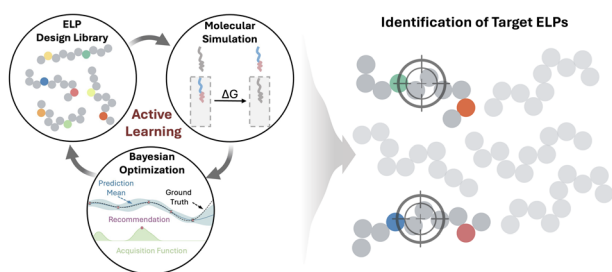
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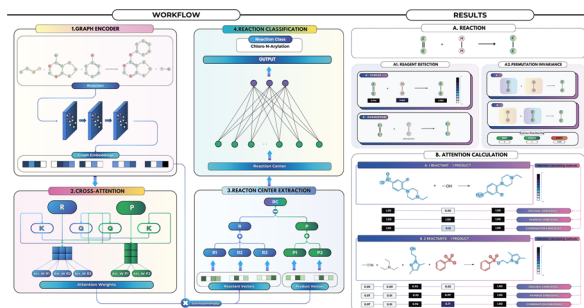
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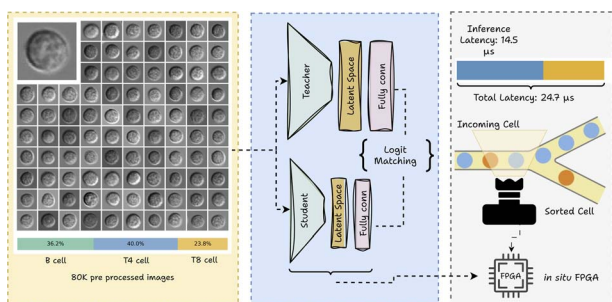
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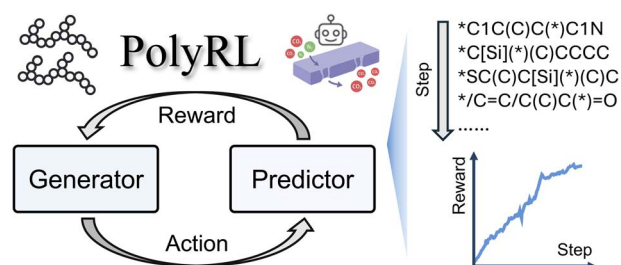
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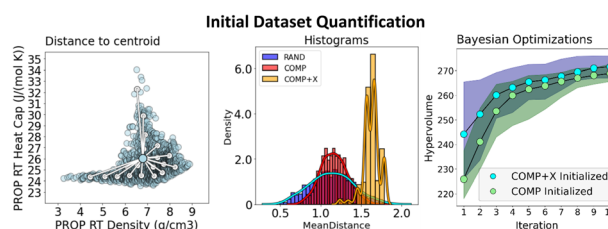
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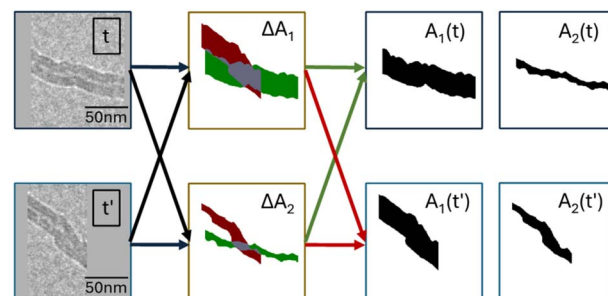
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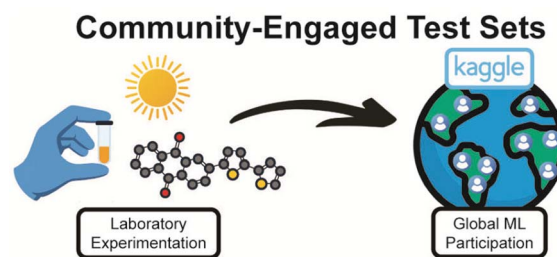
Yushuo Niu, Tianyu Li, Yuanyuan Zhu and Qian Yang\*



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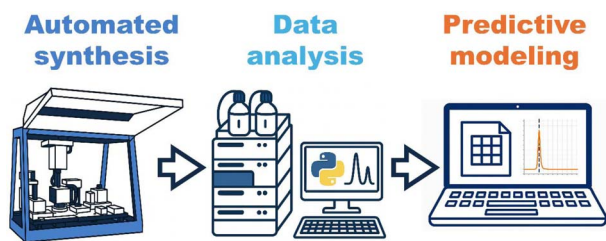
Jason L. Wu, David M. Friday, Changyun Hwang, Seungjoo Yi, Tiara C. Torres-Flores, Martin D. Burke, Ying Diao, Charles M. Schroeder and Nicholas E. Jackson\*



Democratizing Chemical Discovery



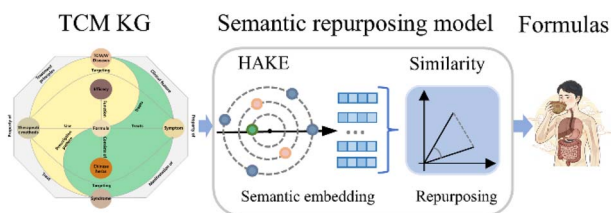
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Sitanan Sartyoungkul, Balasubramaniyan Sakthivel, Pavel Sidorov\* and Yuuya Nagata\*

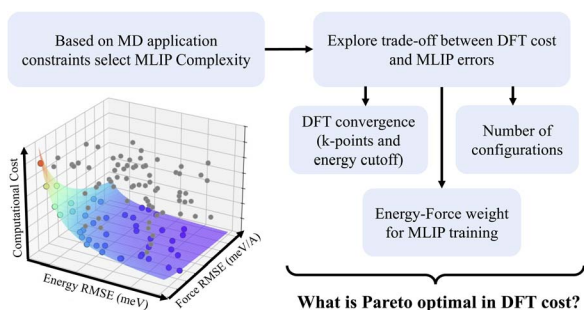
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Xu Dong, Wenyan Zhao, Feifei Li, LiHong Hu,\* Hongzhi Li and Guangzhe Li\*

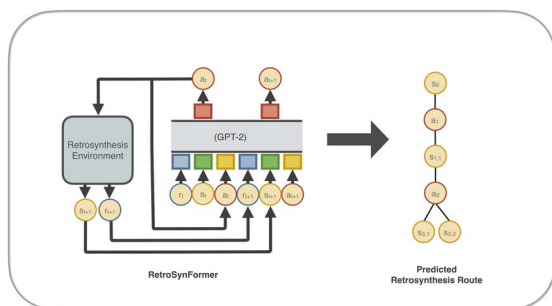
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Ilgar Baghishov,\* Jan Janssen, Graeme Henkelman and Danny Perez\*

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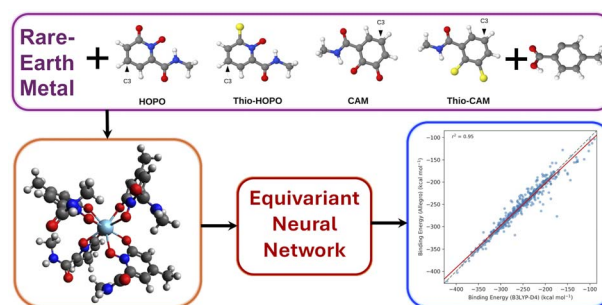
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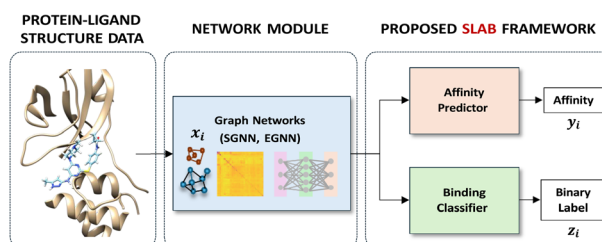
Ankur K. Gupta,\* Caitlin V. Hetherington and Wibe A. de Jong\*



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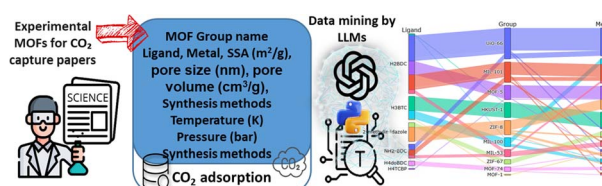
Aditya Ranganath,\* Hyojin Kim, Heesung Shim and Jonathan E. Allen



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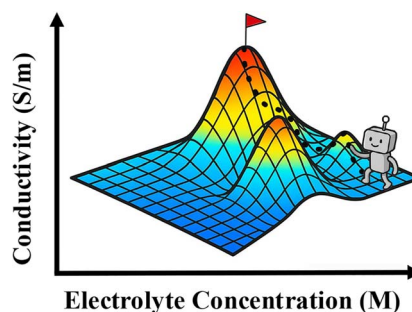
Hossein Mashhadimoslem,\* Mohammad Ali Abdol, Kourosh Zanganeh, Ahmed Shafeen, Encheng Liu, Sohrab Zendejboudi, Ali Elkamel and Aiping Yu\*



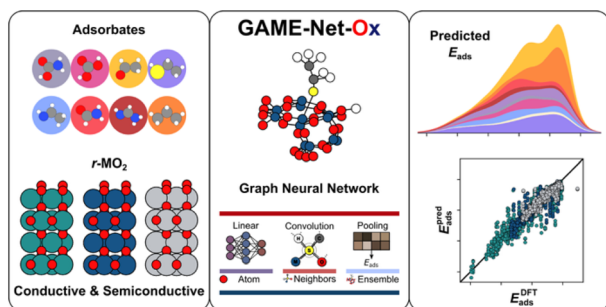
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### BRINE: a cost-effective electrochemical self-driving laboratory for accelerated discovery of high-performance electrolytes

Mohamadreza Ramezani, Poulomi Nandi, Pablo Antonio De La Fuente-Moreno and Majid Beidaghi\*



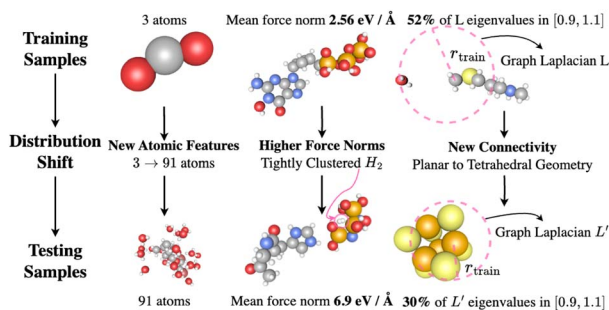
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Thomas Van Hout, Oliver Loveday, Jordi Morales-Vidal, Santiago Morandi and Núria López\*

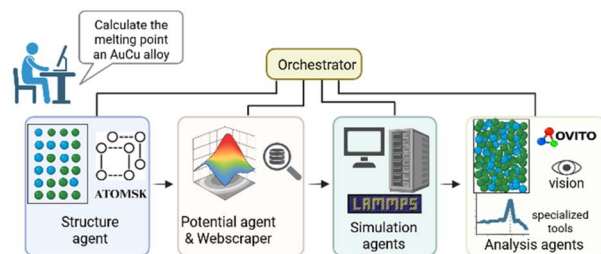
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Tobias Kreiman\* and Aditi S. Krishnapriyan

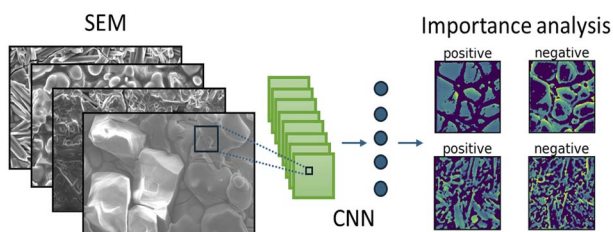
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Kento Murakami, Yudai Yamaguchi, Yo Kato, Kazuki Ishikawa, Naoto Tanibata, Hayami Takeda,\* Masanobu Nakayama\* and Masayuki Karasuyama



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**Correction: Advancing mutagenicity predictions in drug discovery with an explainable few-shot deep learning framework**

Luis H. M. Torres,\* Sofia M. da Silva, Joel P. Arrais, Catarina Pimentel and Bernardete Ribeiro

