

Digital Discovery

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See Ge Lei *et al.*, pp. 1257–1272. Image reproduced by permission of Ge Lei from *Digital Discovery*, 2024, 3, 1257. Image generated with Adobe Firefly.



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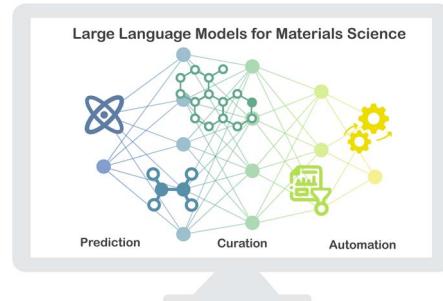
See Antoni Forner-Cuenca *et al.*, pp. 1292–1307. Image reproduced by permission of Maxime van der Heijden and Antoni Forner-Cuenca from *Digital Discovery*, 2024, 3, 1292.

PERSPECTIVE

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Materials science in the era of large language models: a perspective

Ge Lei, Ronan Docherty and Samuel J. Cooper*

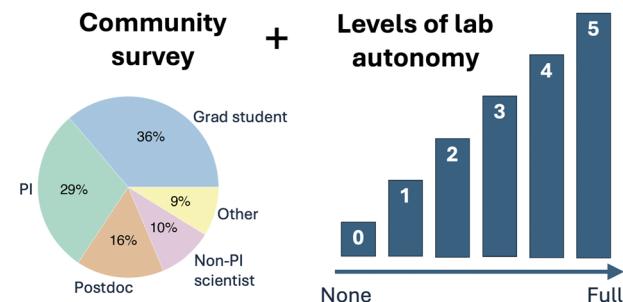


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Autonomous laboratories for accelerated materials discovery: a community survey and practical insights

Linda Hung,* Joyce A. Yager, Danielle Monteverde, Dave Baiocchi, Ha-Kyung Kwon,* Shijing Sun* and Santosh Suram*



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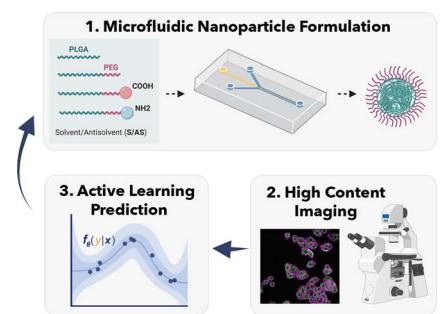
Fundamental questions
Elemental answers

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Machine learning-guided high throughput nanoparticle design

Ana Ortiz-Perez, Derek van Tilborg, Roy van der Meel, Francesca Grisoni* and Lorenzo Albertazzi*

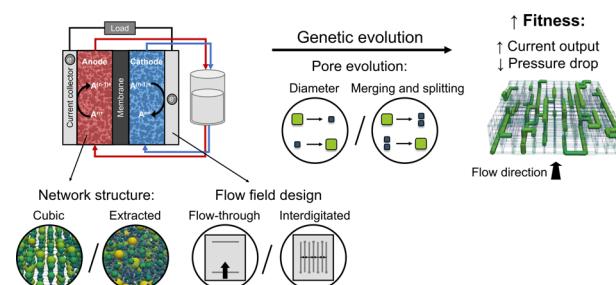


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A versatile optimization framework for porous electrode design

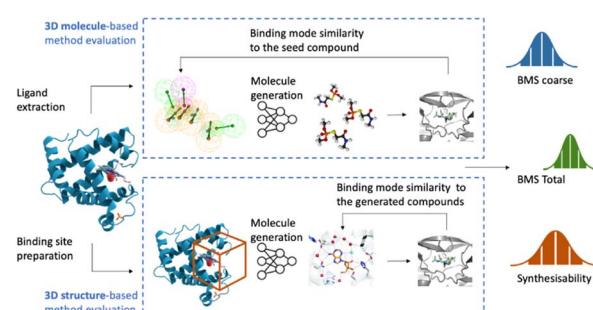
Maxime van der Heijden, Gabor Szendrei, Victor de Haas and Antoni Forner-Cuenca*



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Zygimantas Jocys,* Joanna Grundy and Katayoun Farrahi

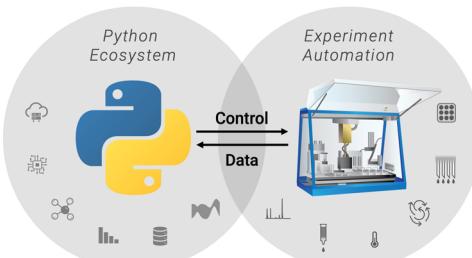


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ChemsPyd: an open-source python interface for Chemspeed robotic chemistry and materials platforms

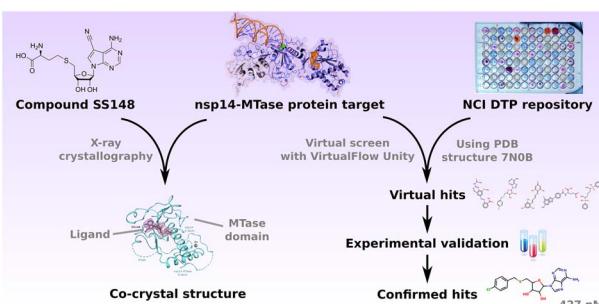
Martin Seifrid, Felix Strieth-Kalthoff, Mohammad Haddadnia, Tony C. Wu, Emre Alca, Leticia Bodo, Sebastian Arellano-Rubach, Naruki Yoshikawa, Marta Skreta, Rachel Keunen and Alán Aspuru-Guzik*

ChemsPyd: A Python API for Chemspeed Robotics



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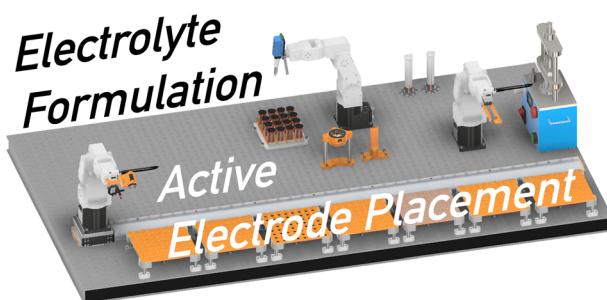
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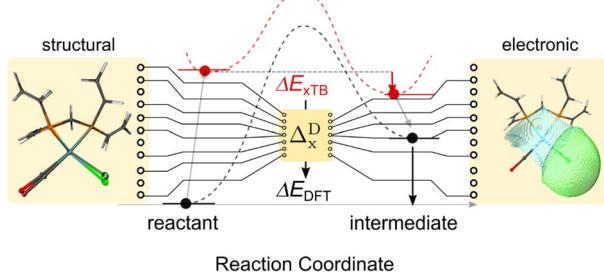
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Apples to apples: shift from mass ratio to additive molecules per electrode area to optimize Li-ion batteries

Bojing Zhang,* Leon Merker, Monika Vogler, Fuzhan Rahamanian and Helge S. Stein*

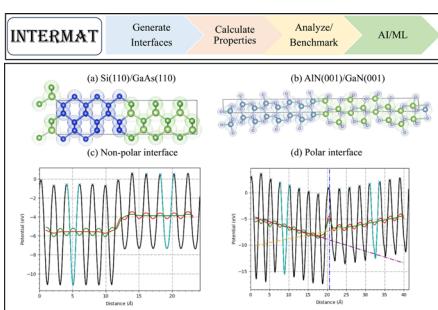
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Tailoring phosphine ligands for improved C–H activation: insights from Δ -machine learning

Tianbai Huang, Robert Geitner,* Alexander Croy* and Stefanie Gräfe*

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Kamal Choudhary* and Kevin F. Garrity

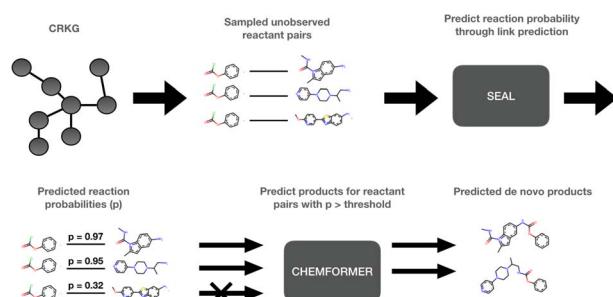


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Expanding the chemical space using a chemical reaction knowledge graph

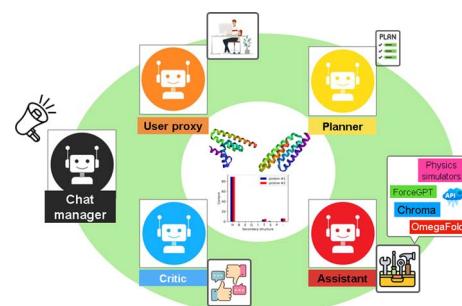
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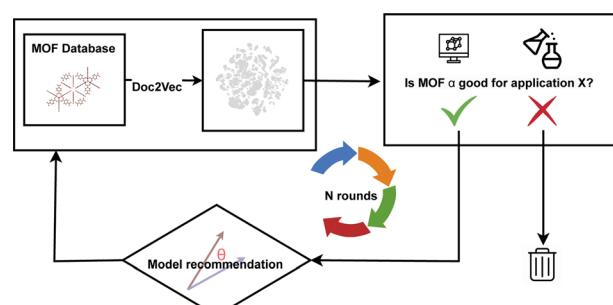
Alireza Ghafarollahi and Markus J. Buehler*



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Deep learning-based recommendation system for metal–organic frameworks (MOFs)

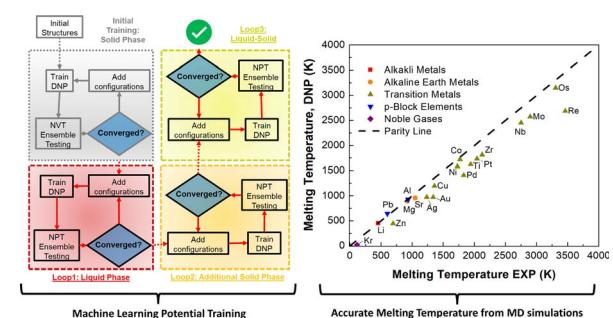
Xiaoqi Zhang, Kevin Maik Jablonka and Berend Smit*



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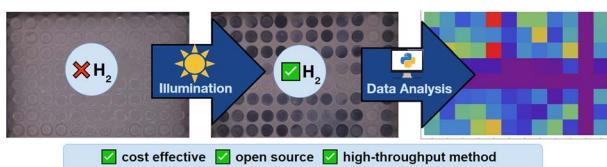
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Christopher M. Andolina and Wissam A. Saidi*



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**High throughput methodology for investigating green hydrogen generating processes using colorimetric detection films and machine vision**

Savannah Talledo, Andrew Kubaney, Mitchell A. Baumer, Keegan Pietrak and Stefan Bernhard*

