

Digital Discovery

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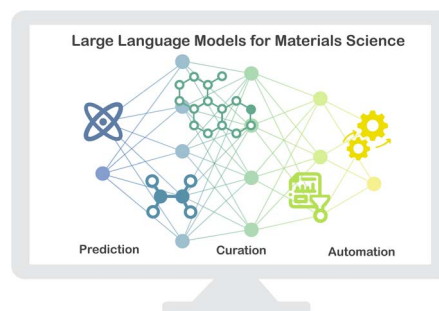
Inside cover
See Antoni Forner-Cuenca *et al.*, pp. 1292–1307. Image reproduced by permission of Maxime van der Heijden and Antoni Forner-Cuenca from *Digital Discovery*, 2024, 3, 1292.

PERSPECTIVE

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

Ge Lei, Ronan Docherty and Samuel J. Cooper*

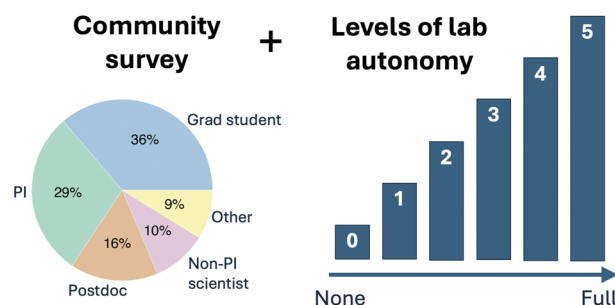


OPINION

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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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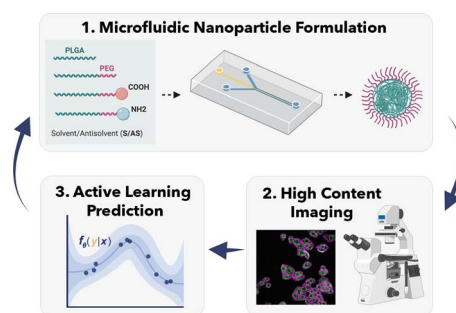
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Fundamental questions
Elemental answers

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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*

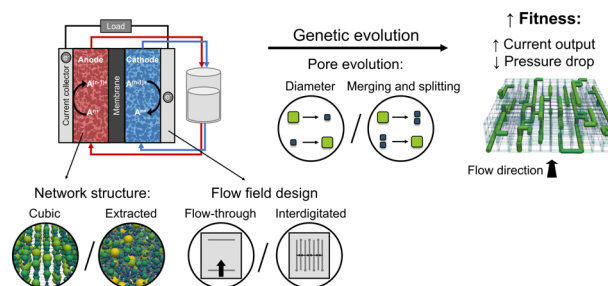


PAPERS

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A versatile optimization framework for porous electrode design

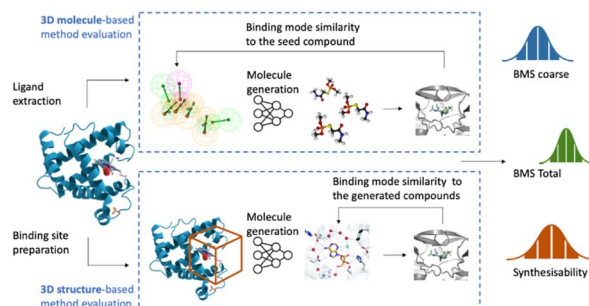
Maxime van der Heijden, Gabor Szendrei, Victor de Haas and Antoni Forner-Cuenca*



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Zygimantas Jocys*, Joanna Grundy and Katayoun Farrahi

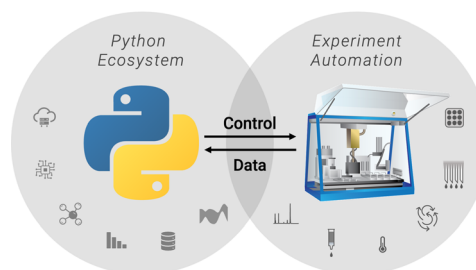


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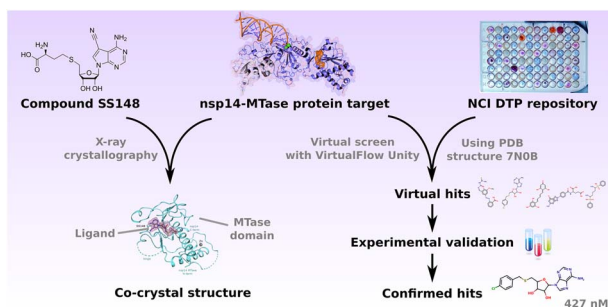
Chemspyd: an open-source python interface for Chemspeed robotic chemistry and materials platforms

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



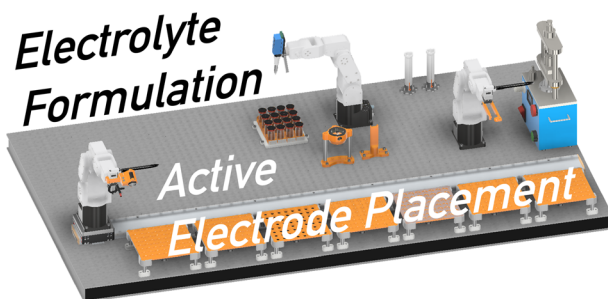
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Application of established computational techniques to identify potential SARS-CoV-2 Nsp14-MTase inhibitors in low data regimes

A. Nigam, M. F. D. Hurley, F. Li, E. Konkořová, M. Klíma, J. Trylčová, R. Pollice, S. S. Çinaroğlu, R. Levin-Konigsberg, J. Handjaya, M. Schapira, I. Chau, S. Perveen, H.-L. Ng, H. Ü. Kaniskan, Y. Han, S. Singh, C. Gorgulla, A. Kundaje, J. Jin, V. A. Voelz, J. Weber, R. Nencka, E. Boura, M. Vedadi* and A. Aspuru-Guzik*

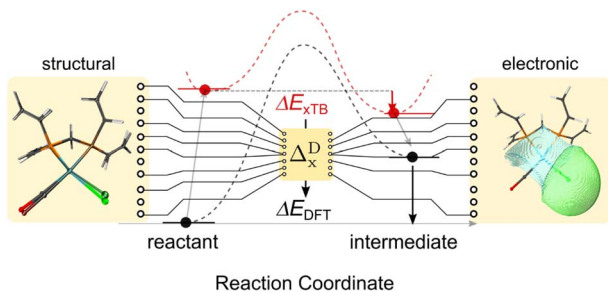
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Apples to apples: shift from mass ratio to additive molecules per electrode area to optimize Li-ion batteries

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

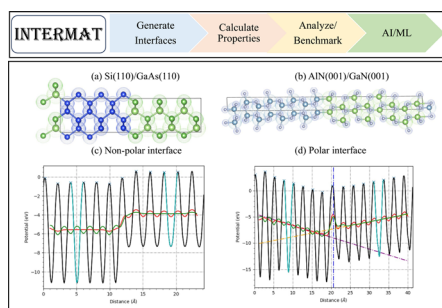
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Tailoring phosphine ligands for improved C–H activation: insights from Δ -machine learning

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

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InterMat: accelerating band offset prediction in semiconductor interfaces with DFT and deep learning

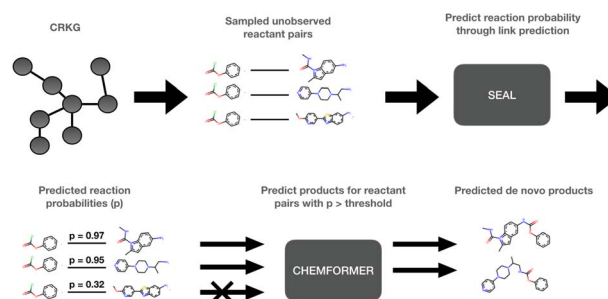
Kamal Choudhary* and Kevin F. Garrity



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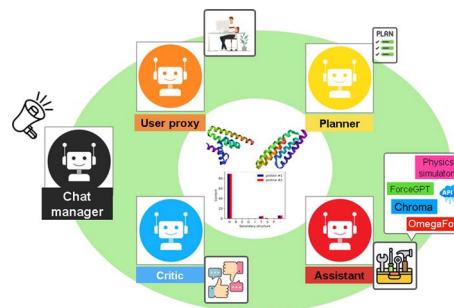
Emma Rydholm,^{*} Tomas Bastys, Emma Svensson, Christos Kannas, Ola Engkvist and Thierry Kogej



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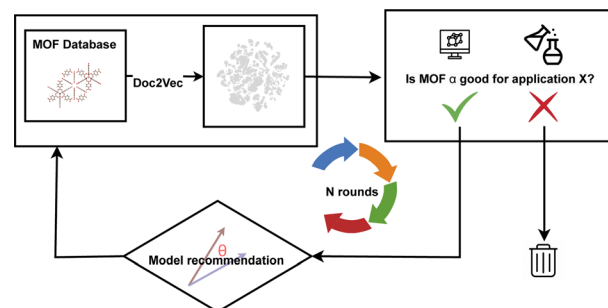
Alireza Ghafarollahi and Markus J. Buehler^{*}



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

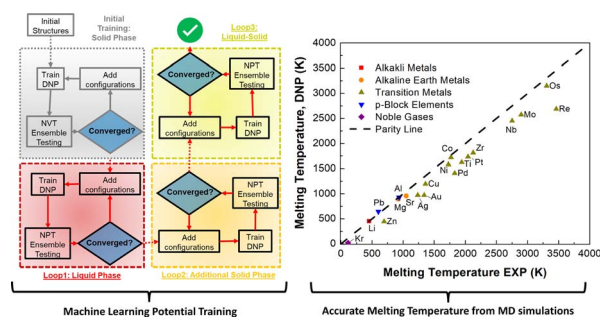
Xiaoqi Zhang, Kevin Maik Jablonka and Berend Smit^{*}



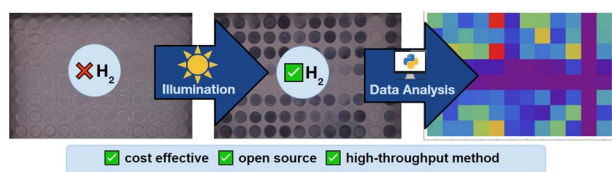
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Predicting melting temperatures across the periodic table with machine learning atomistic potentials

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*

