

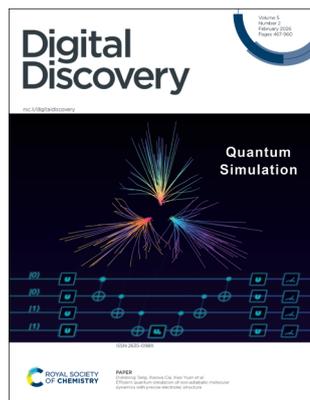
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See Diandong Tang, Xiaoxia Cai, Xiao Yuan *et al.*, pp. 548–570. Image reproduced by permission of Tianyi Li from *Digital Discovery*, 2026, 5, 548.



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Accelerating catalytic advancements through the precision of high-throughput experiments & calculations

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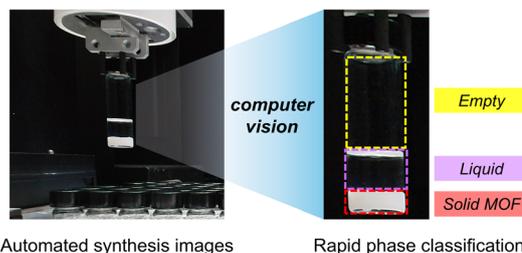
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Image-based characterization for high-throughput materials discovery

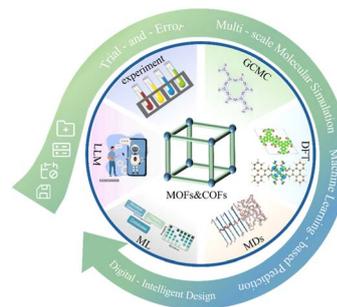


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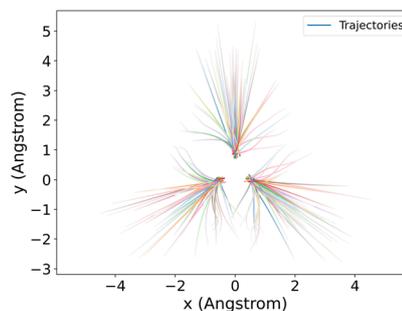


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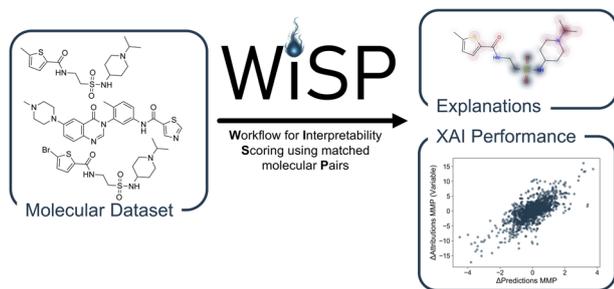
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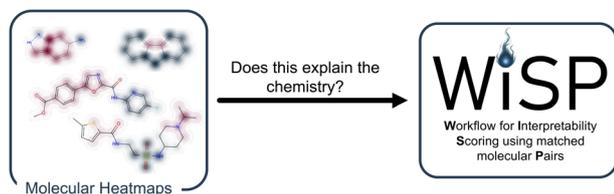
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When machine learning models learn chemistry I: quantifying explainability with matched molecular pairs

Kerrin Janssen, Jan M. Wollschläger, Jonny Proppe* and Andreas H. Göller*

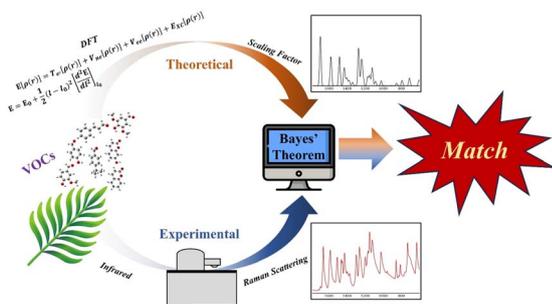
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Kerrin Janssen, Jan M. Wollschläger, Jonny Proppe* and Andreas H. Göller*

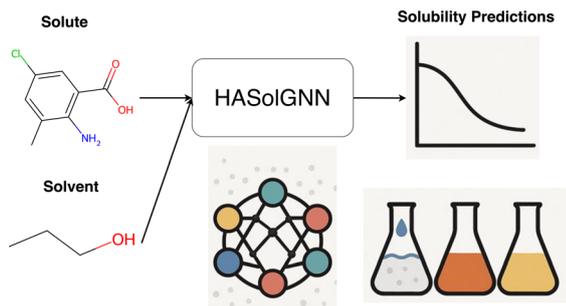
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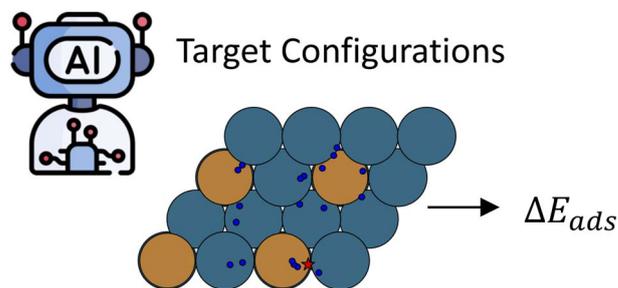
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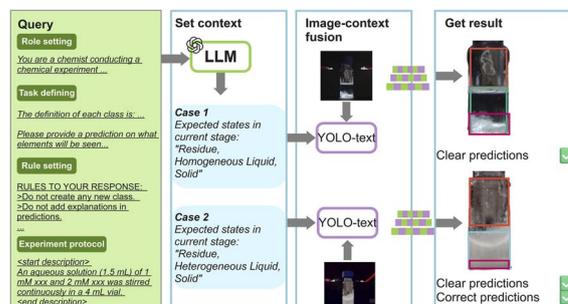
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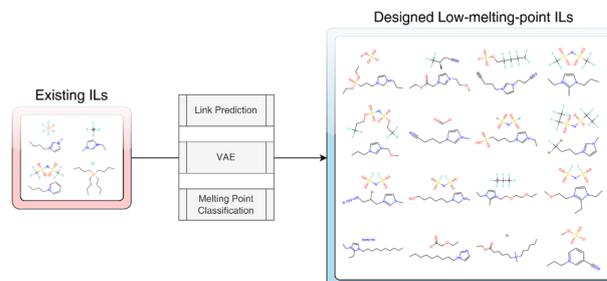
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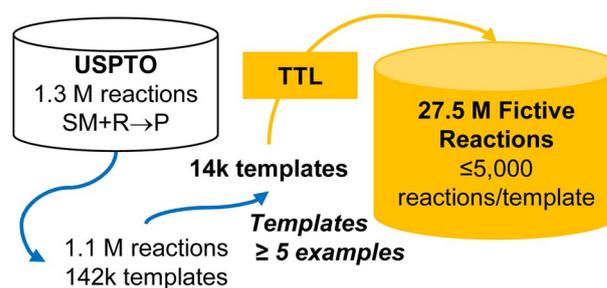
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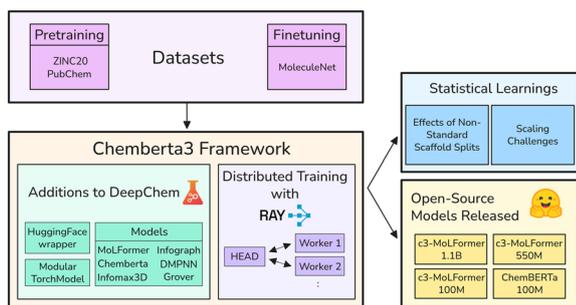
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Data augmentation in a triple transformer loop retrosynthesis model

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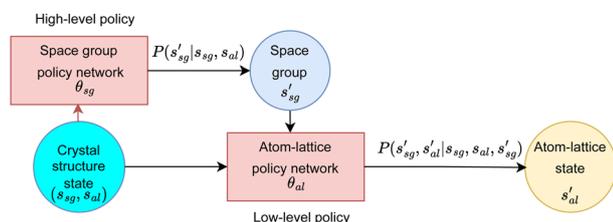
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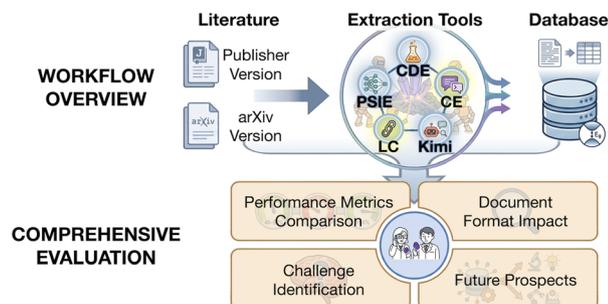
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Efficient symmetry-aware materials generation via hierarchical generative flow networks

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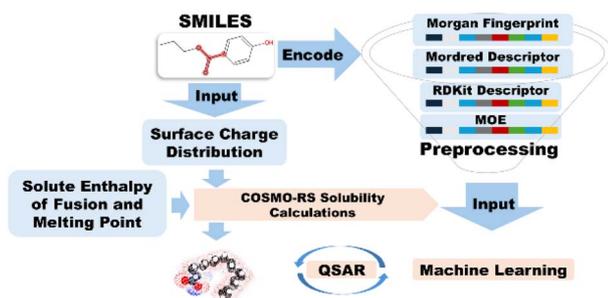
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A case study on hybrid machine learning and quantum-informed modelling for solubility prediction of drug compounds in organic solvents

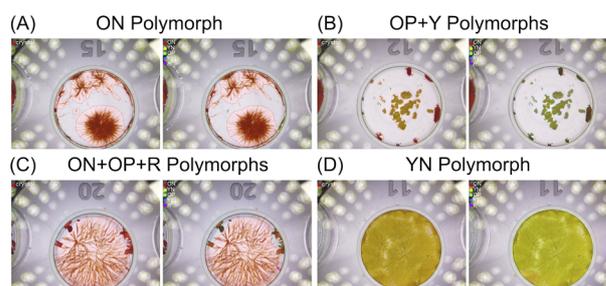
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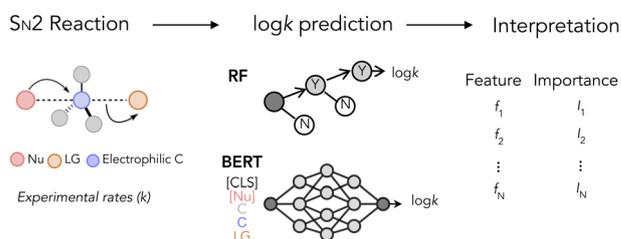
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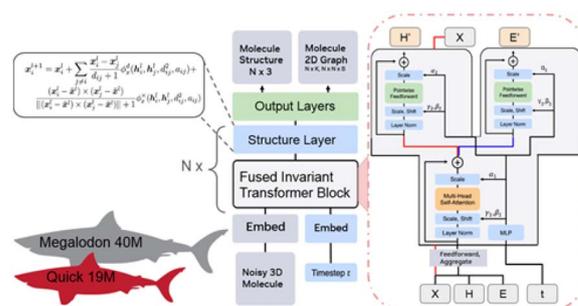
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Applications of modular co-design for de novo 3D molecule generation

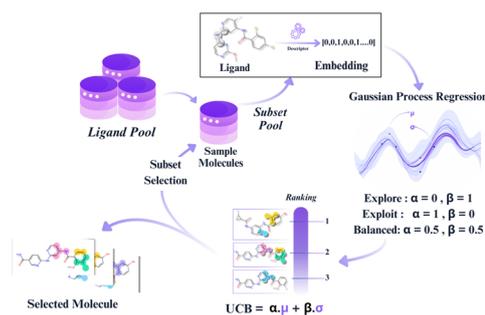
Danny Reidenbach,* Filipp Nikitin,* Olexandr Isayev and Saeed Gopal Paliwal



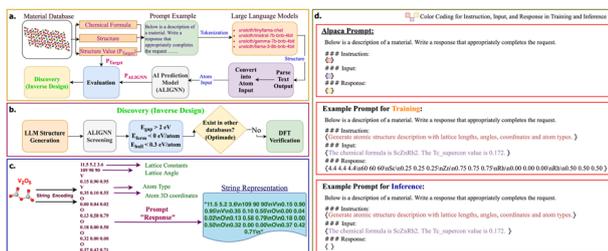
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Explainable active learning framework for ligand binding affinity prediction

Satya Pratik Srivastava, Rohan Gorantla, Sharath Krishna Chundru, Claire J. R. Winkelman, Antonia S. J. S. Mey* and Rajeev Kumar Singh*



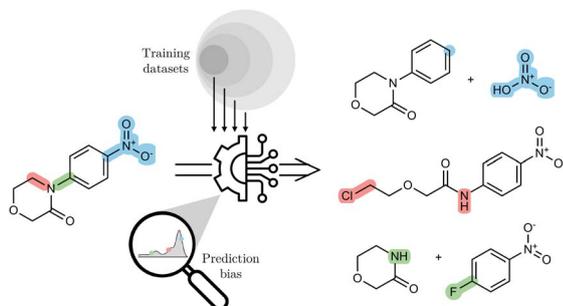
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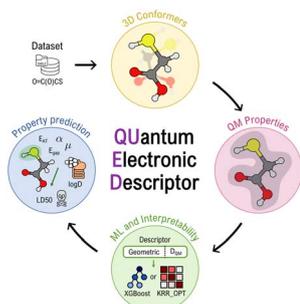
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An exploration of dataset bias in single-step retrosynthesis prediction

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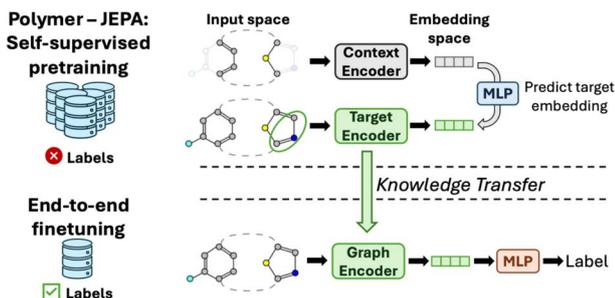
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Alejandra Hinostroza Caldas, Artem Kokorin,
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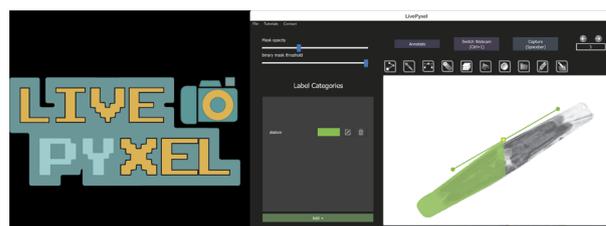


Joint embedding predictive architecture for self-supervised pretraining on polymer molecular graphs

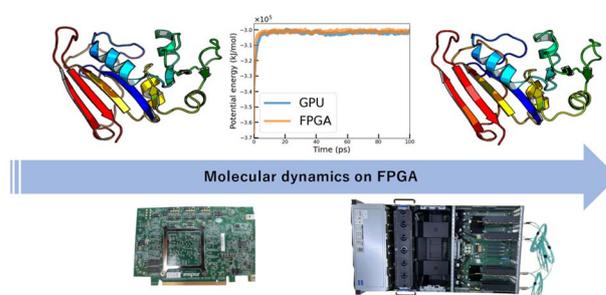
Francesco Piccoli, Gabriel Vogel and Jana M. Weber*



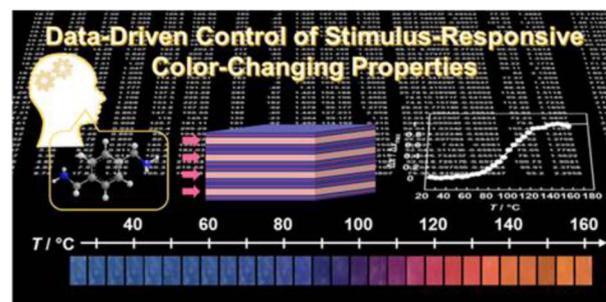
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LivePyxel: accelerating image annotations with a Python-integrated webcam live streamingUriel Garcilazo-Cruz,^{*} Joseph O. Okeme and Rodrigo A. Vargas-Hernández^{*}

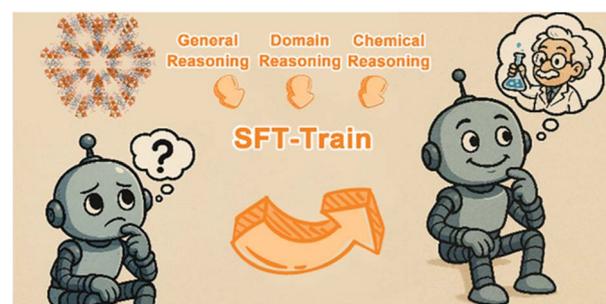
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Molecular dynamics simulations accelerated on FPGA with high-bandwidth memoryJing Xiao, Jinfeng Chen, Ye Ding, You Xu and Jing Huang^{*}

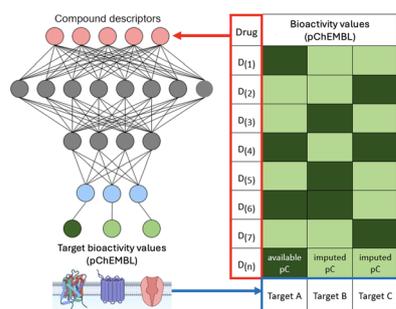
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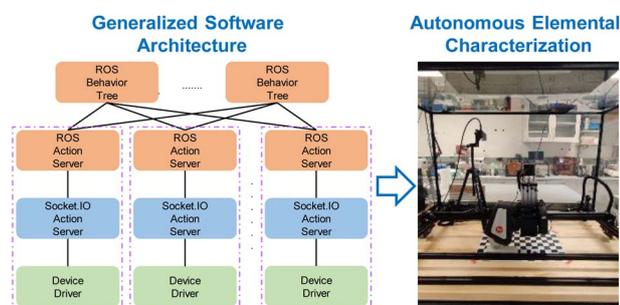
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A multi-task learning approach for prediction of missing bioactivity values of compounds for the SLC transporter superfamily

Tarik Ćerimagić, Sergey Sosnin and Gerhard F. Ecker*

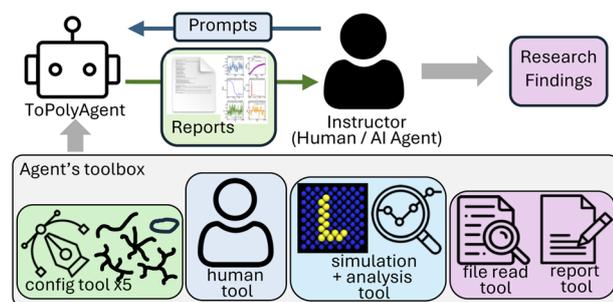
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Autonomous elemental characterization enabled by a low cost robotic platform built upon a generalized software architecture

Xuan Cao,* Yuxin Wu and Michael L. Whittaker*

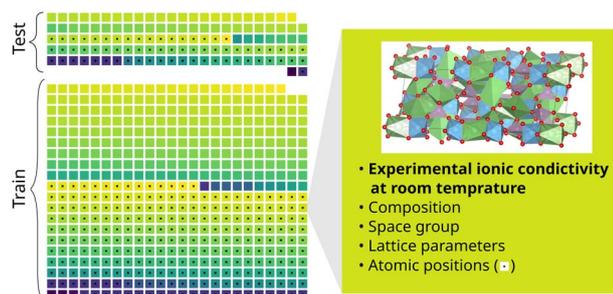
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OBELiX: a curated dataset of crystal structures and experimentally measured ionic conductivities for lithium solid-state electrolytes

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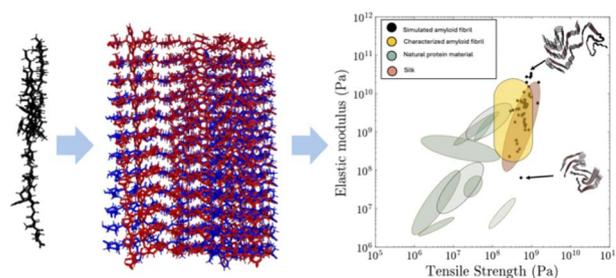


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FiberForge: enabling high-throughput simulations of the mechanical properties of helical fibrils

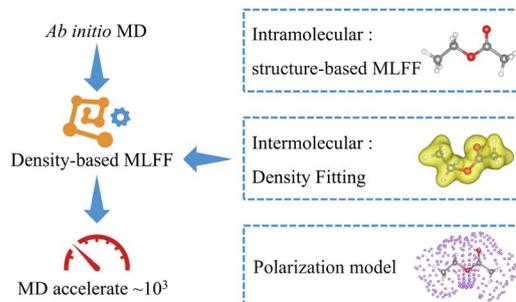
Kieran Nehil-Puleo and Zhongyue John Yang*



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DBMLFF: linear scaling machine learning force fields via electron density decomposition for molecular electrolytes

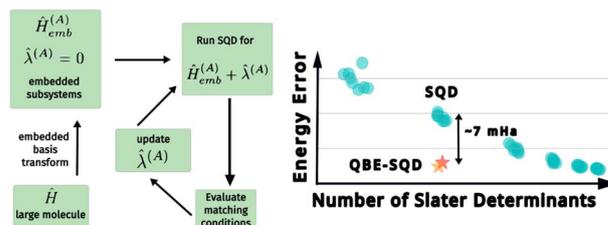
Jie Shen, Chenyu Wang, Libin Chen, Shaoqin Jiang,* Jianhui Chen, Cuilian Wen, Bo Wu, Baisheng Sa* and Lin-Wang Wang*



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Towards utility-scale electronic structure with sample-based quantum bootstrap embedding

Joel Bierman and Yuan Liu*



CORRECTION

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Correction: A case study on hybrid machine learning and quantum-informed modelling for solubility prediction of drug compounds in organic solvents

Weiling Wang, Isabel Cooley, Morgan R. Alexander, Ricky D. Wildman, Anna K. Croft and Blair F. Johnston*

