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See Julia Westermayr *et al.*, pp. 1501–1509. Image reproduced by permission of Hendrik Weiske from *Digital Discovery*, 2026, 5, 1501.



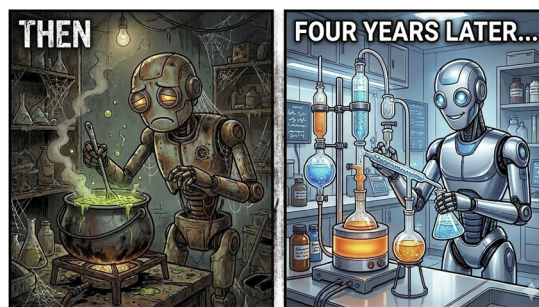
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See DongWook Kim *et al.*, pp. 1510–1521. Image reproduced by permission of DongWook Kim from *Digital Discovery*, 2026, 5, 1510. Image generated with Adobe Firefly.

PERSPECTIVE

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Looking back and to the future after four-plus years of language in chemistry

Glen M. Hocky* and Andrew D. White*

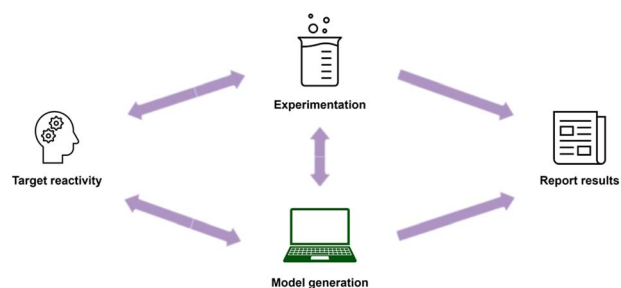


REVIEWS

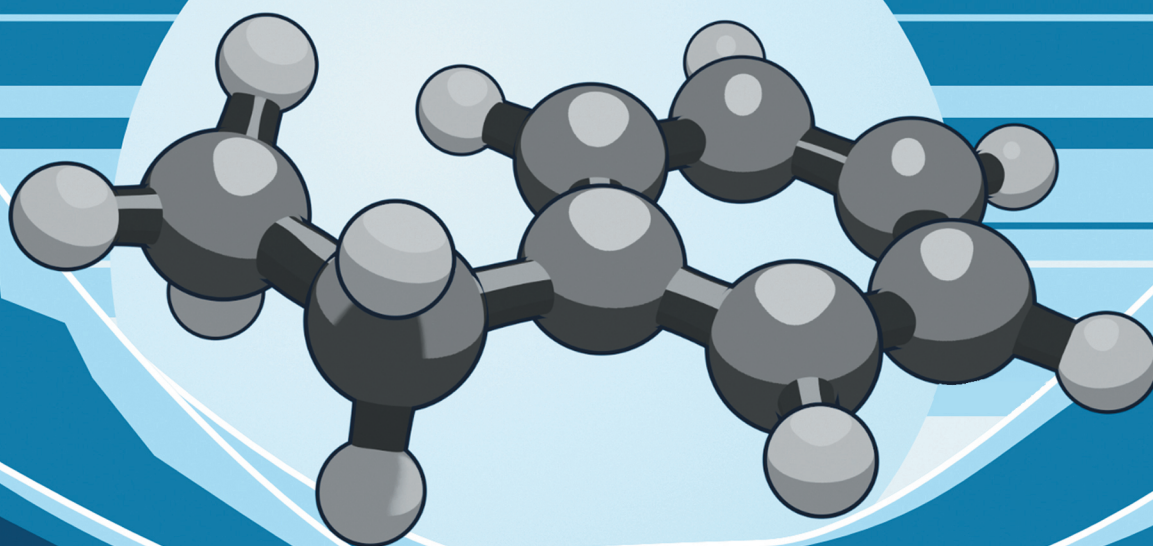
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Reaction optimization through mechanistic insight and predictive modelling

Roger Monreal-Corona,* Anna Pla-Quintana* and Albert Poater*



Cheminformatics, Automation and Machine Learning in Chemistry (CAMLC)



June 2nd-5th, 2026
Zaragoza, Spain

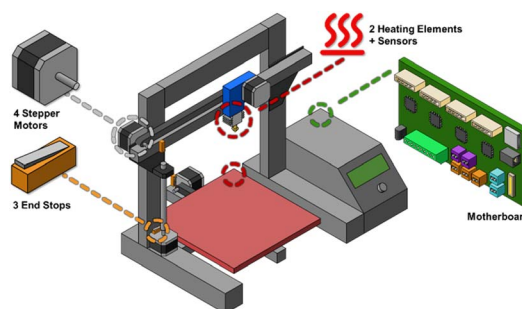


REVIEWS

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Hacking 3D printers as laboratory robots

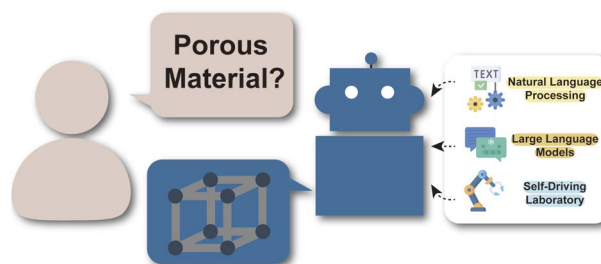
Sander Baas, Nessa Carson and Vittorio Saggiomo*



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Large language models for porous materials: from text mining to autonomous laboratory

Seunghee Han, Taeun Bae, Junho Kim, Younghun Kim and Jihan Kim*

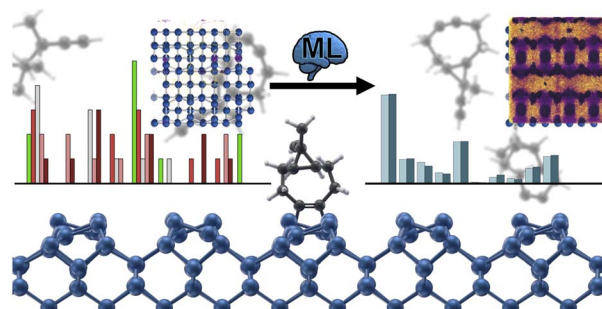


PAPERS

1501

Statistics makes a difference: machine learning adsorption dynamics of functionalized cyclooctyne on Si(001) at DFT accuracy

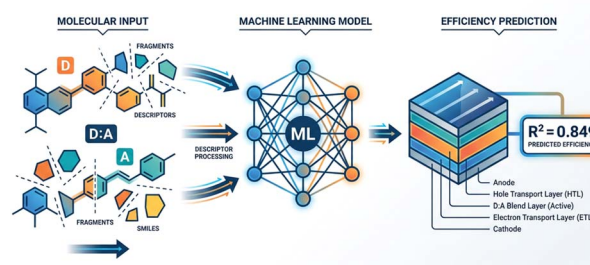
Hendrik Weiske, Rhyan Barrett, Ralf Tonner-Zech, Patrick Melix and Julia Westermayr*



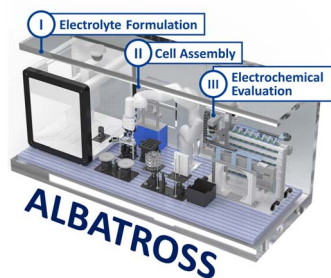
1510

Structure-guided machine learning for efficiency prediction of organic photovoltaics using experimentally informed molecular descriptors

JuHyun Lee, HyoJin Ban, HyunIl Seo, HangKen Lee, Fiza Arshad and DongWook Kim*



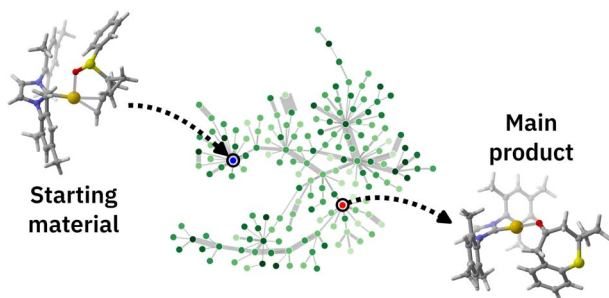
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ALBATROSS: a robotised system for high-throughput electrolyte screening *via* automated electrolyte formulation, coin-cell fabrication, and electrochemical evaluation

Hyun-Gi Lee, Jaekyeong Han, Minjun Kwon, Hyeonuk Kwon, Jooha Park, Hoe Jin Hah and Dong-Hwa Seo*

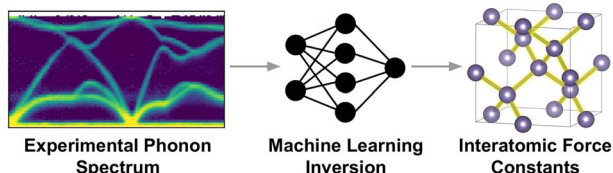
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Distilling system complexity to enable unbiased and predictive computational reaction investigations

Raphaël Robidas* and Claude Y. Legault*

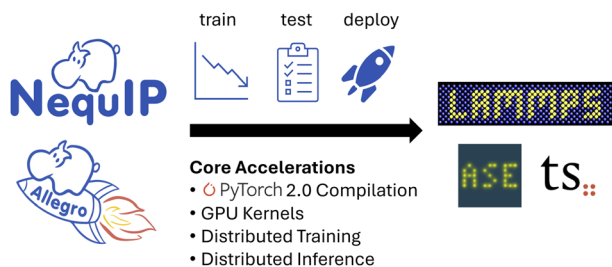
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Machine learning inversion of interatomic force constants from single-crystal inelastic neutron scattering

Aiden Sable, Bander Linjawi, Kyle Bradbury, Jordan Malof and Olivier Delaire*

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High-performance training and inference for deep equivariant interatomic potentials

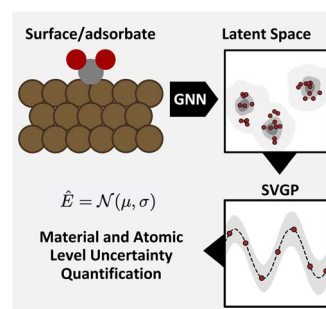
Chuin Wei Tan, Marc L. Descoteaux, Mit Kotak, Gabriel de Miranda Nascimento, Seán R. Kavanagh, Laura Zichi, Menghang Wang, Aadit Saluja, Yizhong R. Hu, Tess Smidt, Anders Johansson, William C. Witt, Boris Kozinsky* and Albert Musaelian*



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Deep graph kernel learning for material & atomic level uncertainty quantification in adsorption energy prediction

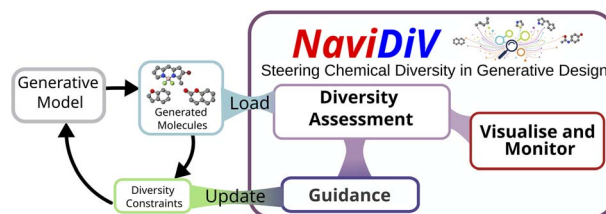
Osman Mamun, Chenlu Yang and Shuwen Yue*



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NaviDiv: a web app for monitoring chemical diversity in generative molecular design

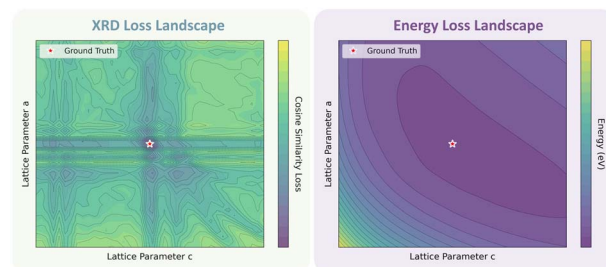
Mohammed Azzouzi,* Thanapat Worakul and Clémence Corminboeuf



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The loss landscape of powder X-ray diffraction-based structure optimization is too rough for gradient descent

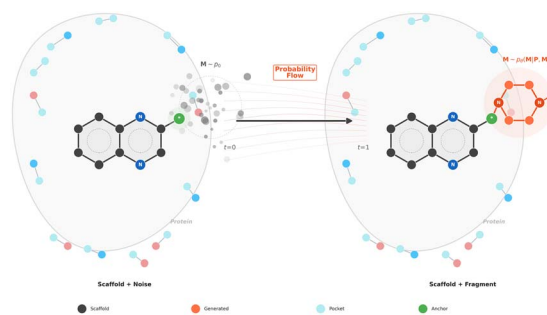
Nofit Segal, Akshay Subramanian, Mingda Li, Benjamin Kurt Miller and Rafael Gómez-Bombarelli*



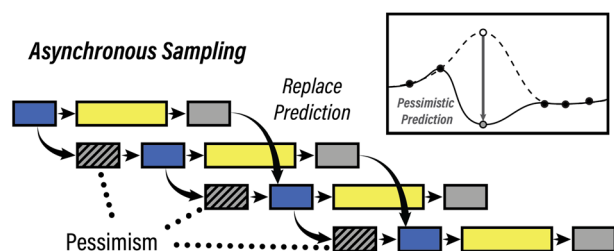
1600

Coupled fragment-based generative modeling with stochastic interpolants

Tuan Le,* Yanfei Guan, Djork-Arné Clevert and Kristof T. Schütt



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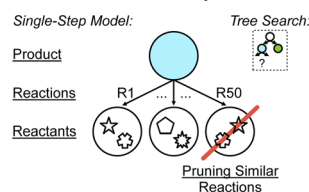


Pessimistic asynchronous sampling in high-cost Bayesian optimization

Amanda A. Volk,^{*} Kristofer G. Reyes, Jeffrey G. Ethier and Luke A. Baldwin^{*}

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Synthesis Planning in Reaction Space



Route Finding Success

Online Search vs. Self-Play

Search Robustness

Changing Stock Availability

Route Diversity

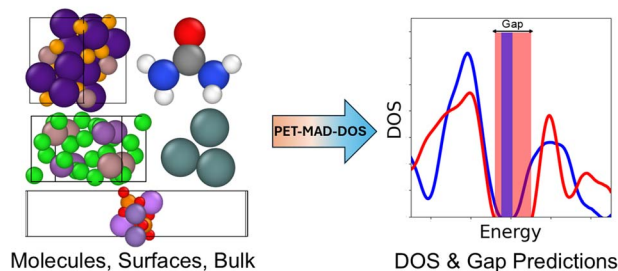
Solution Space Coverage

Synthesis planning in reaction space: a study on success, robustness and diversity

Alan Kai Hassen,^{*} Helen Lai, Samuel Genheden, Mike Preuss and Djork-Arné Clevert

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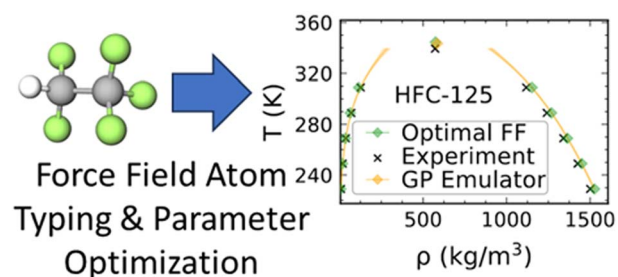
PET-MAD-DOS: Universal Transformer for Electronic States



A universal machine learning model for the electronic density of states

Wei Bin How, Pol Febrer, Sanggyu Chong, Arslan Mazitov, Filippo Bigi, Matthias Kellner, Sergey Pozdnyakov and Michele Ceriotti^{*}

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Development of accurate transferable hydrofluorocarbon refrigerant force fields using a machine learning and optimization approach

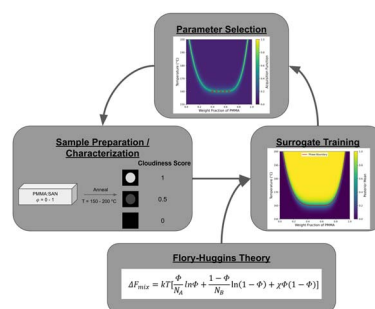
Montana N. Carlozo, Ning Wang, Alexander W. Dowling^{*} and Edward J. Maginn^{*}



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Using Flory–Huggins-informed human-in-the-loop Bayesian optimization to map the phase diagram of polymer blends

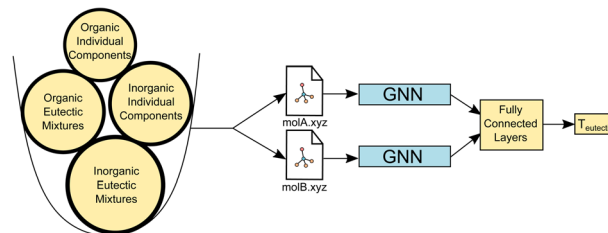
Justin C. Hughes, Dylan J. York, Kevin G. Yager, Chinedum O. Osuji and Russell J. Composto*



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Siamese graph neural networks for melting temperature prediction of molten salt eutectics

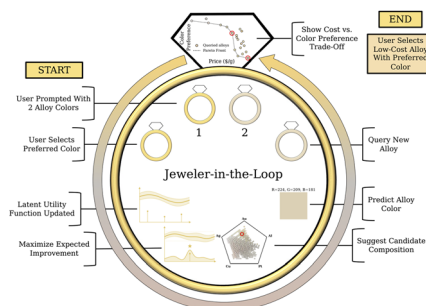
Nila Mandal, James Maniscalco, Mark Aindow and Qian Yang*



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Jeweler-in-the-loop: personalized alloy color optimization via preference-based BO

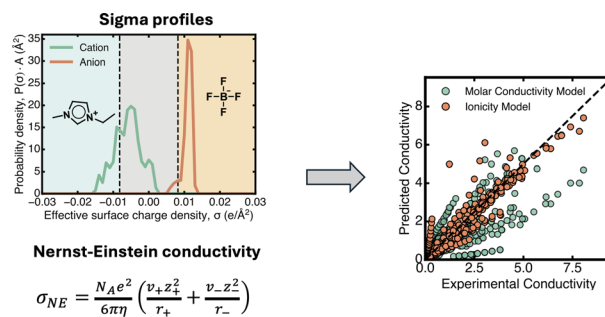
Chase Katz,* Ting-Yu Yang, Parker King, Md Shafiqul Islam, Brent Vela and Raymundo Arróyave



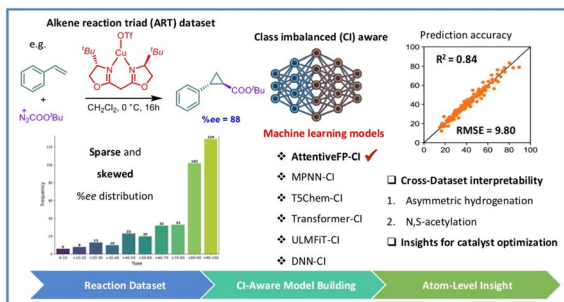
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Exploring the deviation from Nernst–Einstein conductivity in ionic liquids using machine learning

Aditi Seshadri, Lyndon T. M. Hess and Shuwen Yue*



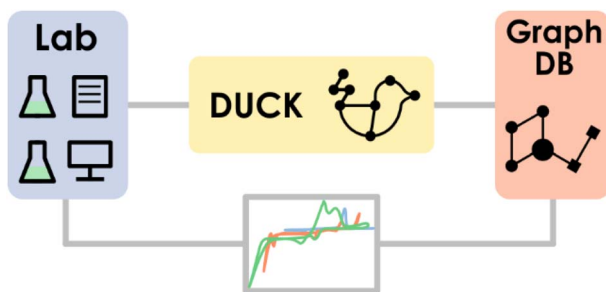
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Machine learning models for catalytic asymmetric reactions of simple alkenes: from enantioselectivity predictions to chemical insights

Ajnabiul Hoque, Nupur Jain, Divya Chenna and Raghavan B. Sunoj*

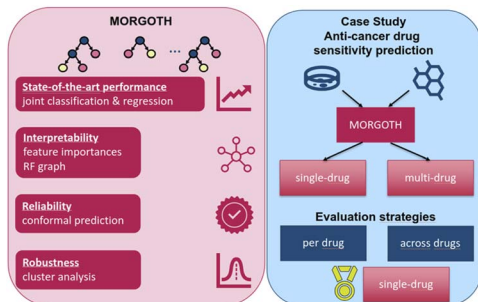
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Database utility for cyclovoltammetry knowledge (DUCK): unified platform for electrochemical data

Diego Garay-Ruiz, Sergio Pablo-García, Han Hao and Marisol Martín-González*

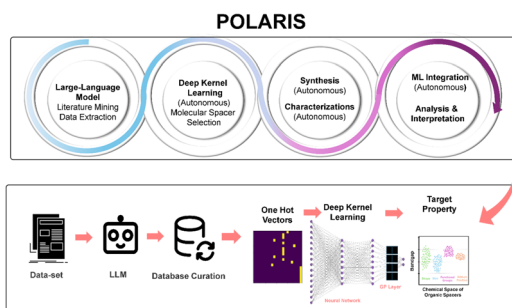
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Increasing trustworthiness of machine learning-based drug sensitivity prediction with a multivariate random forest approach

Lisa-Marie Rolli,* Lea Eckhart, Lutz Herrmann, Andrea Volkamer, Hans-Peter Lenhof and Kerstin Lenhof

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POLARIS: perovskite optimization using LLM-assisted refinement and intelligent screening

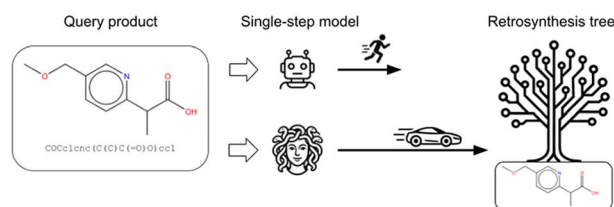
Jordan Marshall, Sheryl L. Sanchez, Rushik Desai, Elham Foadian, Utkarsh Pratiush, Arun Mannodi-Kanakkithodi, Sergei V. Kalinin and Mahshid Ahmadi*



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Fast and scalable retrosynthetic planning with a transformer neural network and speculative beam search

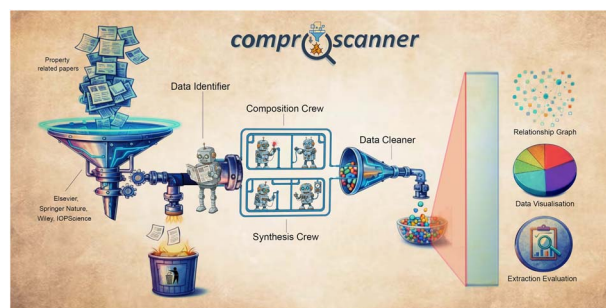
Natalia Andronova, Mikhail Andronov,*
Jürgen Schmidhuber, Michael Wand and
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ComProScanner: a multi-agent based framework for composition-property structured data extraction from scientific literature

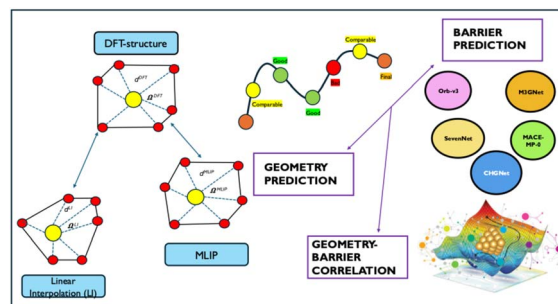
Aritra Roy,* Enrico Grisan, John Buckeridge* and
Chiara Gattinoni*



1809

Evaluation of foundational machine learned interatomic potentials for migration barrier predictions

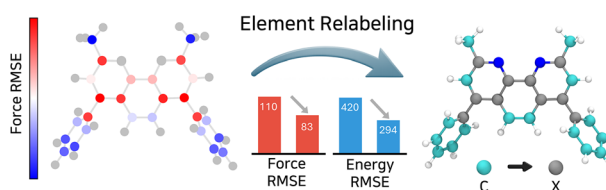
Achintha Krishna Bheemaguli, Penghao Xiao* and
Gopalakrishnan Sai Gautam*



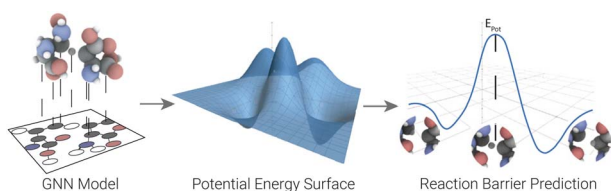
1820

Enhancing high-dimensional neural network potential accuracy in OLED systems via element relabeling

Yonghwan Yun, Dongmin Park, Junyoung Choi,
Dong Shin Choi and Yousung Jung*



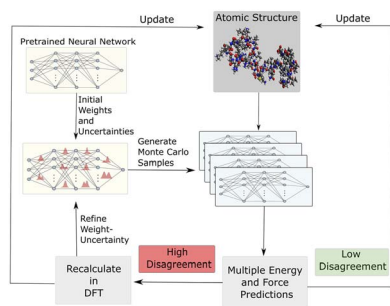
1831



Learning potential energy surfaces of hydrogen atom transfer reactions in peptides

Marlen Neubert, Patrick Reiser, Frauke Gräter* and Pascal Friederich*

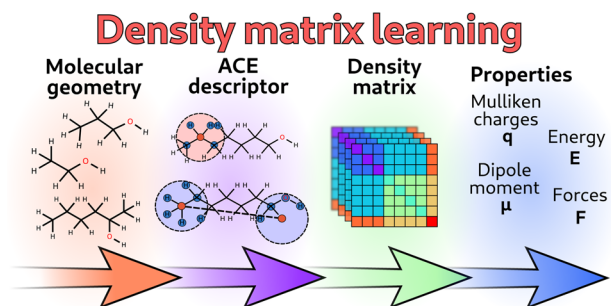
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On-the-fly fine-tuning of foundational neural network potentials: a Bayesian neural network approach

Tim Rensmeyer,* Denis Kramer and Oliver Niggemann

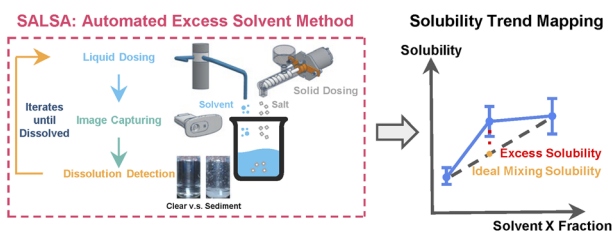
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A symmetry-preserving and transferable representation for learning the Kohn–Sham density matrix

Liwei Zhang,* Patrizia Mazzeo, Michele Nottoli, Edoardo Cignoni, Lorenzo Cupellini and Benjamin Stamm

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SALSA: a low-cost self-driving lab modular add-on for salt solubility assessment for battery electrolytes

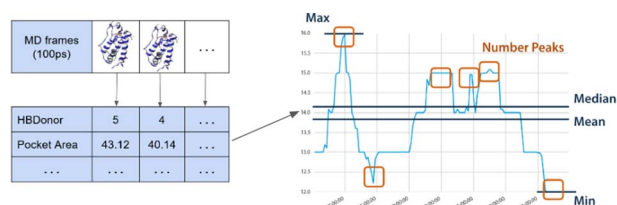
Tianyi Zhang, Hongyi Lin, Yuhan Chen and Venkatasubramanian Viswanathan*



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Assessment of molecular dynamics time series descriptors in protein–ligand affinity prediction

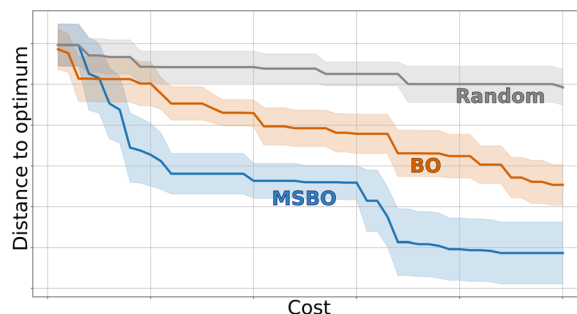
Jakub Poziemski, Artur Yurkevych and Pawel Siedlecki*



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Multi-stage Bayesian optimisation for dynamic decision-making in self-driving labs

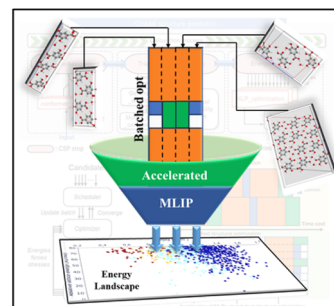
Luca Torresi and Pascal Friederich*



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Integrating machine learning interatomic potentials with batched optimization for crystal structure prediction

Chengxi Zhao,* Zhaojia Ma, Dingrui Fan, Siyu Hu, Leping Wang, Feng Hua, Weile Jia, En Shao,* Guangming Tan,* Jun Jiang* and Linjiang Chen*



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InSpecLearn4SDL: interpretable spectral features predict conductivity in self-driving doped conjugated polymer labs

Ankush Kumar Mishra, Jacob P. Mauthe, Nicholas Luke, Aram Amassian* and Baskar Ganapathysubramanian*

