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See Stanley Lo, Sterling G. Baird, Taylor D. Sparks, Alán Aspuru-Guzik et al., pp. 842–868.
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Inside cover

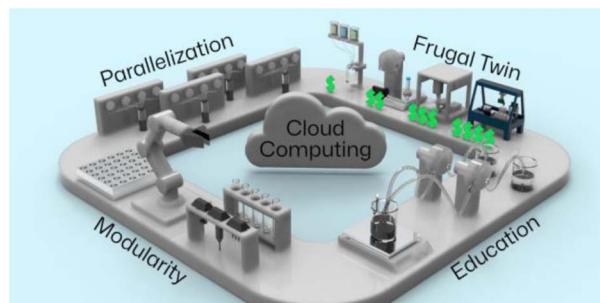
See Mingjian Wen et al., pp. 869–882. Image reproduced by permission of Mingjian Wen from *Digital Discovery*, 2024, 3, 869.

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Review of low-cost self-driving laboratories in chemistry and materials science: the "frugal twin" concept

Stanley Lo,* Sterling G. Baird,* Joshua Schrier, Ben Blaiszik, Nessa Carson, Ian Foster, Andrés Aguilar-Granda, Sergei V. Kalinin, Benji Maruyama, Maria Politi, Helen Tran, Taylor D. Sparks* and Alán Aspuru-Guzik*

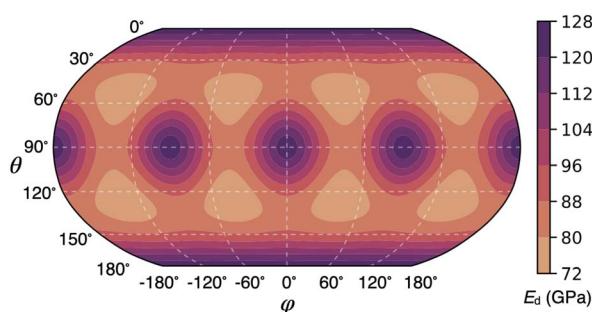


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An equivariant graph neural network for the elasticity tensors of all seven crystal systems

Mingjian Wen,* Matthew K. Horton, Jason M. Munro, Patrick Huck and Kristin A. Persson





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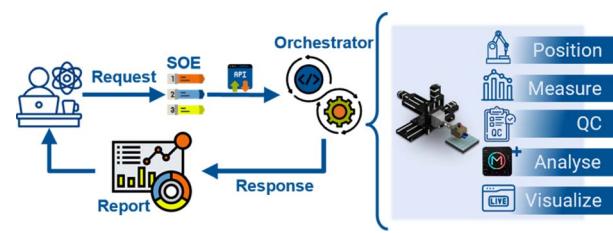


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Autonomous millimeter scale high throughput battery research system

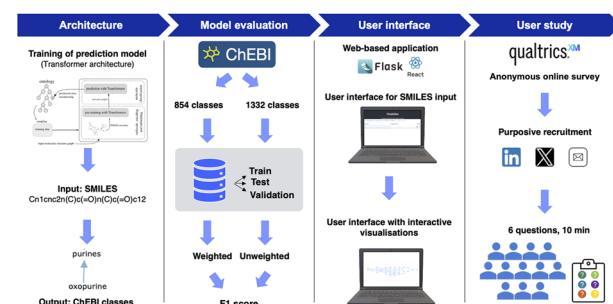
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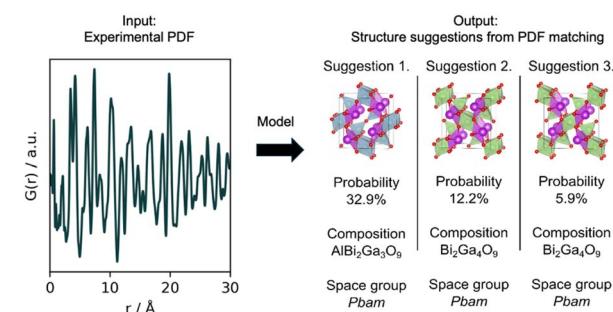
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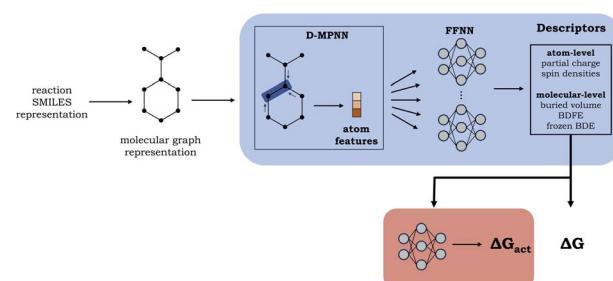
Emil T. S. Kjær, Andy S. Anker, Andrea Kirsch, Joakim Lajer, Olivia Aalling-Frederiksen, Simon J. L. Billinge* and Kirsten M. Ø. Jensen*



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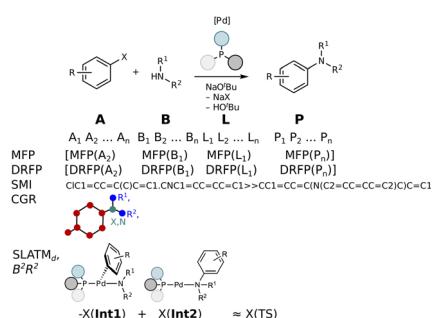
Repurposing quantum chemical descriptor datasets for on-the-fly generation of informative reaction representations: application to hydrogen atom transfer reactions

Javier E. Alfonso-Ramos, Rebecca M. Neeser and Thijs Stuyver*



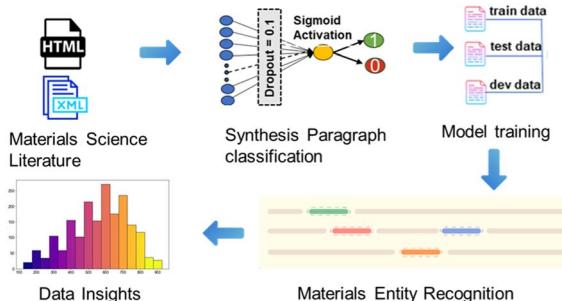
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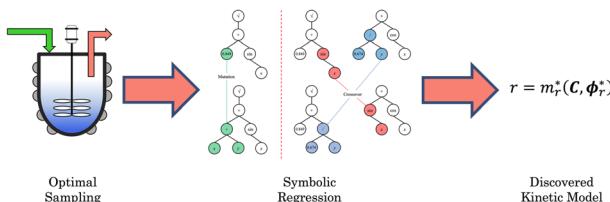
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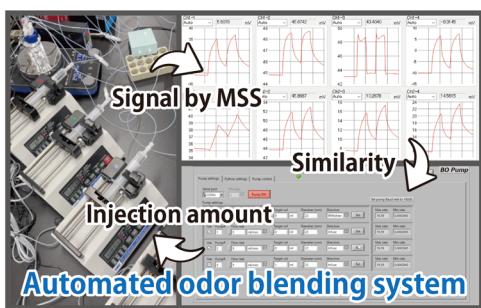
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Yota Fukui, Kosuke Minami,* Kota Shiba, Genki Yoshikawa, Koji Tsuda* and Ryo Tamura*

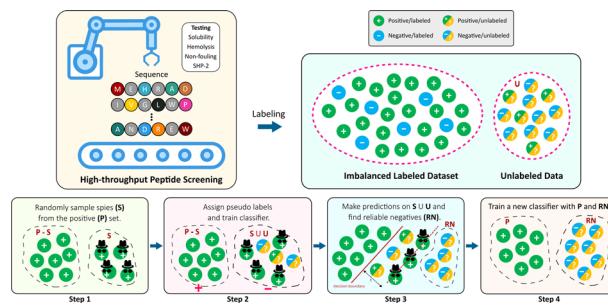


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Learning peptide properties with positive examples only

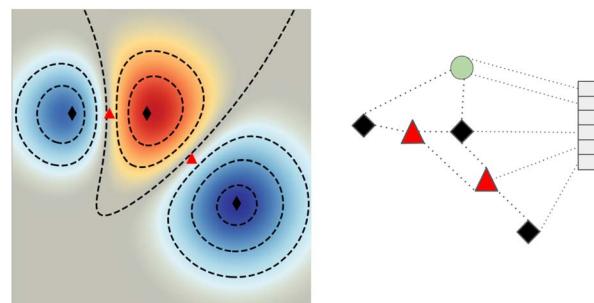
Mehrad Ansari and Andrew D. White*



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High-throughput quantum theory of atoms in molecules (QTAIM) for geometric deep learning of molecular and reaction properties

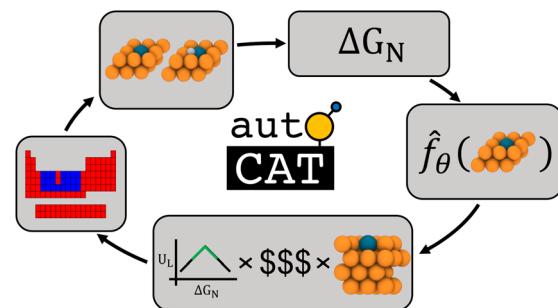
Santiago Vargas,* Winston Gee and Anastassia Alexandrova*



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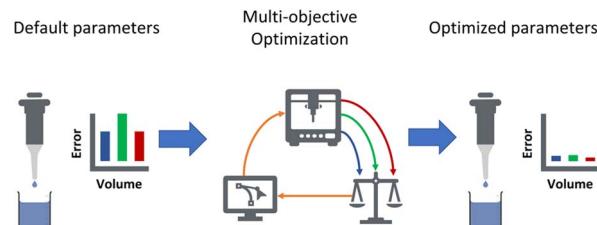
Lance Kavalsky, Vinay I. Hegde, Bryce Meredig and Venkatasubramanian Viswanathan*



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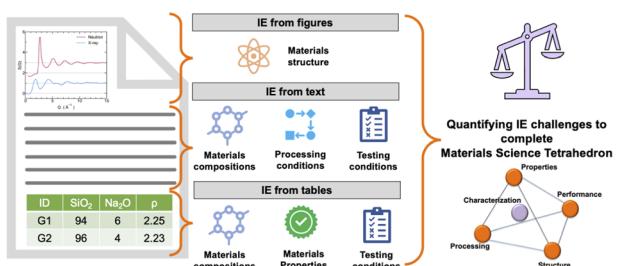
Optimization of liquid handling parameters for viscous liquid transfers with pipetting robots, a "sticky situation"

Pablo Quijano Velasco,* Kai Yuan Andre Low, Chang Jie Leong, Wan Ting Ng, Selina Qiu, Shivam Jhunjhunwala, Bryant Li, Anne Qian, Kedar Hippalgaonkar and Jayce Jian Wei Cheng*



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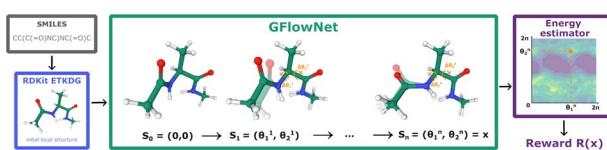
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Reconstructing the materials tetrahedron: challenges in materials information extraction

Kausik Hira, Mohd Zaki, Dhruvil Sheth, Mausam* and N. M. Anoop Krishnan*

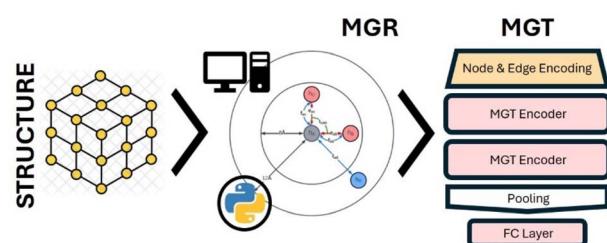
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Towards equilibrium molecular conformation generation with GFlowNets

Alexandra Volokhova,* Michał Koziarski,* Alex Hernández-García, Cheng-Hao Liu, Santiago Miret, Pablo Lemos, Luca Thiede, Zichao Yan, Alán Aspuru-Guzik and Yoshua Bengio

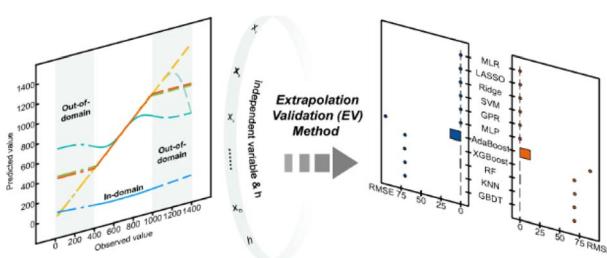
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Molecular graph transformer: stepping beyond ALIGNN into long-range interactions

Marco Anselmi, Greg Slabaugh,* Rachel Crespo-Otero* and Devis Di Tommaso*

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Extrapolation validation (EV): a universal validation method for mitigating machine learning extrapolation risk

Mengxian Yu, Yin-Ning Zhou, Qiang Wang and Fangyou Yan*



CORRECTIONS

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Correction: Tackling data scarcity with transfer learning: a case study of thickness characterization from optical spectra of perovskite thin films

Siyu Isaac Parker Tian, Zekun Ren, Selvaraj Venkataraj, Yuanhang Cheng, Daniil Bash, Felipe Oviedo, J. Senthilnath, Vijila Chellappan, Yee-Fun Lim, Armin G. Aberle, Benjamin P. MacLeod, Fraser G. L. Parlane, Curtis P. Berlinguet, Qianxiao Li, Tonio Buonassisi* and Zhe Liu*

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Correction: Predicting small molecules solubility on endpoint devices using deep ensemble neural networks

Mayk Caldas Ramos and Andrew D. White*

