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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
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TUTORIAL REVIEW

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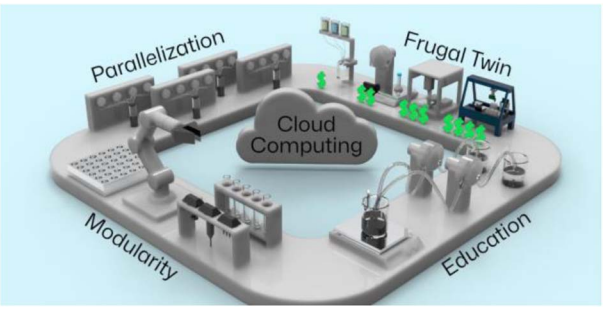
Review of low-cost self-driving laboratories in chemistry and materials science: the "frugal twin" concept

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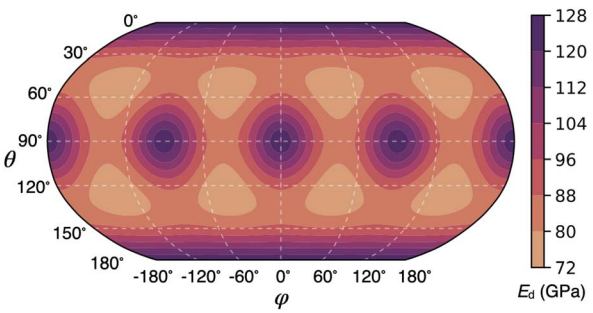
An equivariant graph neural network for the elasticity tensors of all seven crystal systems

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



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PAPERS

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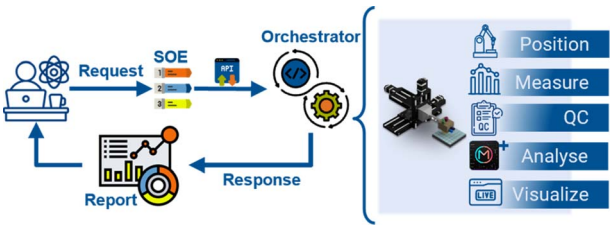
Autonomous millimeter scale high throughput battery research system

Fuzhan Rahmanian,* Stefan Fuchs, Bojing Zhang, Maximilian Fichtner and Helge Sören Stein*



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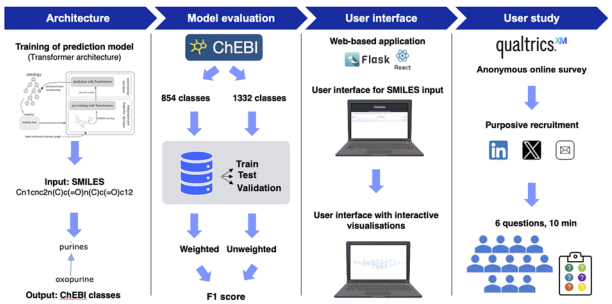
Chebifier: automating semantic classification in ChEBI to accelerate data-driven discovery

Martin Glauer, Fabian Neuhaus, Simon Flügel, Marie Wosny, Till Mossakowski, Adel Memariani, Johannes Schwerdt and Janna Hastings



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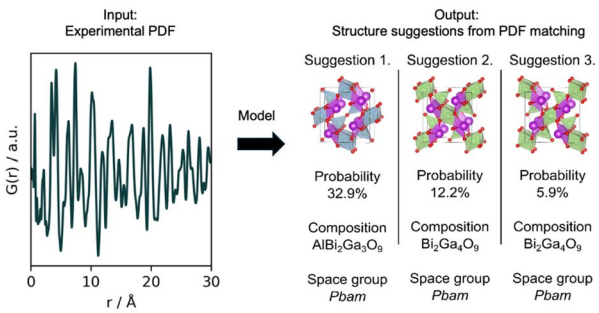
MLstructureMining: a machine learning tool for structure identification from X-ray pair distribution functions

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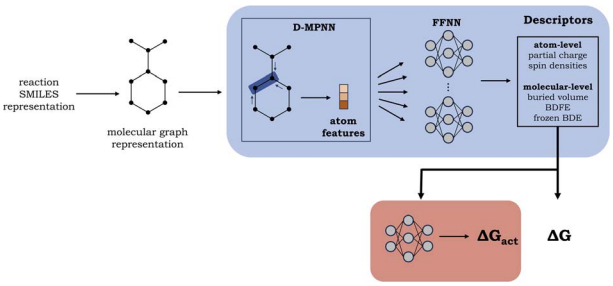
Repurposing quantum chemical descriptor datasets for on-the-fly generation of informative reaction representations: application to hydrogen atom transfer reactions

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



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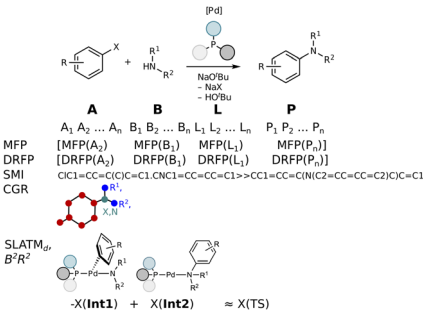

Benchmarking machine-readable vectors of chemical reactions on computed activation barriers

Puck van Gerwen, Ksenia R. Briling, Yannick Calvino Alonso, Malte Franke and Clemence Corminboeuf*

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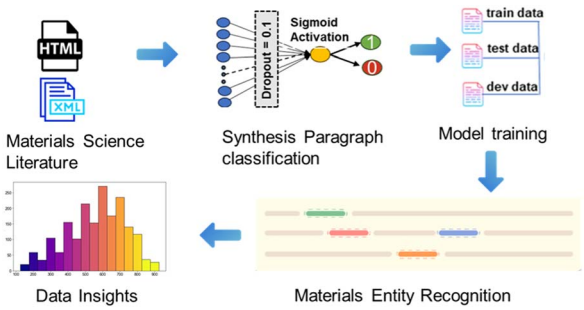

Automated extraction of synthesis parameters of pulsed laser-deposited materials from scientific literature

Rajan Kumar, Ablokit Joshi, Salman A. Khan and Shikhar Misra*

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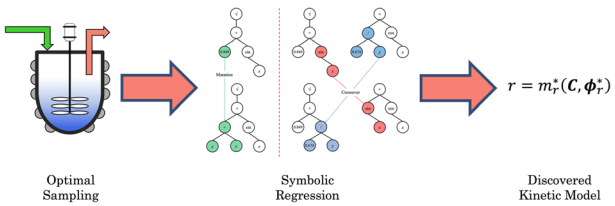

The automated discovery of kinetic rate models – methodological frameworks

Miguel Ángel de Carvalho Servia, Ilya Orson Sandoval, King Kuok (Mimi) Hii, Klaus Hellgardt, Dongda Zhang* and Ehecatl Antonio del Rio Chanona*

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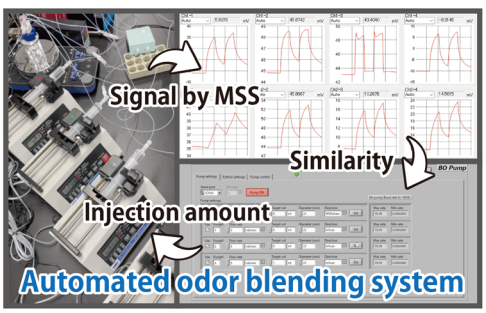

Automated odor-blending with one-pot Bayesian optimization

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

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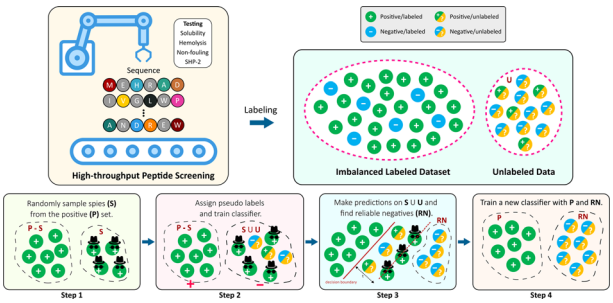
Learning peptide properties with positive examples only

Mehrad Ansari and Andrew D. White*



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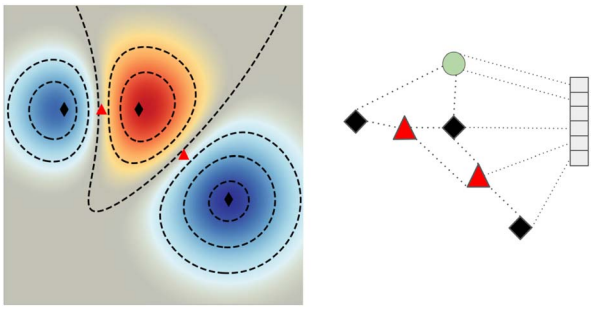
High-throughput quantum theory of atoms in molecules (QTAIM) for geometric deep learning of molecular and reaction properties

Santiago Vargas,* Winston Gee and Anastassia Alexandrova*



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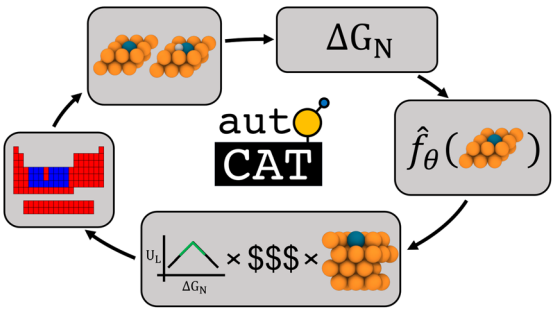
A multiobjective closed-loop approach towards autonomous discovery of electrocatalysts for nitrogen reduction

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



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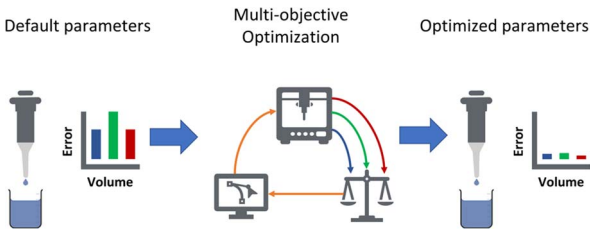
Optimization of liquid handling parameters for viscous liquid transfers with pipetting robots, a "sticky situation"

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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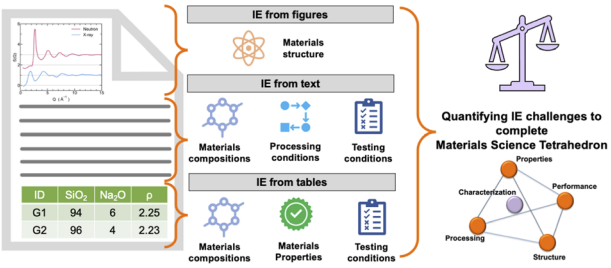

Reconstructing the materials tetrahedron: challenges in materials information extraction

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

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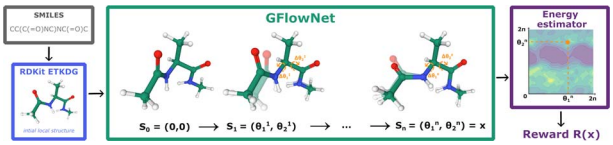

Towards equilibrium molecular conformation generation with GFlowNets

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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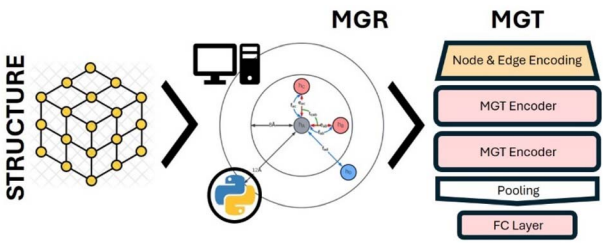

Molecular graph transformer: stepping beyond ALIGNN into long-range interactions

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

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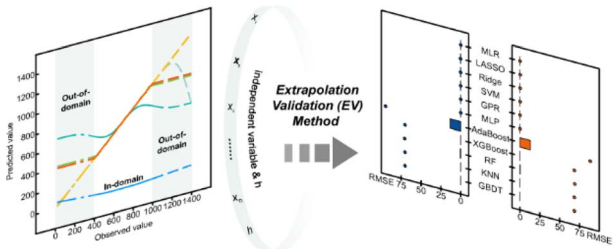

Extrapolation validation (EV): a universal validation method for mitigating machine learning extrapolation risk

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

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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. Berlinguette, 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*

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