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IN THIS ISSUE

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Cover
See Stanley Lo, Sterling G. Baird, Taylor D. Sparks, Alán Aspuru-Guzik *et al.*, pp. 842–868.
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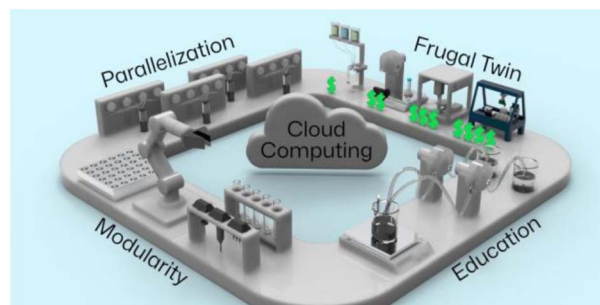
Inside cover
See Mingjian Wen *et al.*, pp. 869–882. Image reproduced by permission of Mingjian Wen from *Digital Discovery*, 2024, 3, 869.

TUTORIAL REVIEW

842

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*

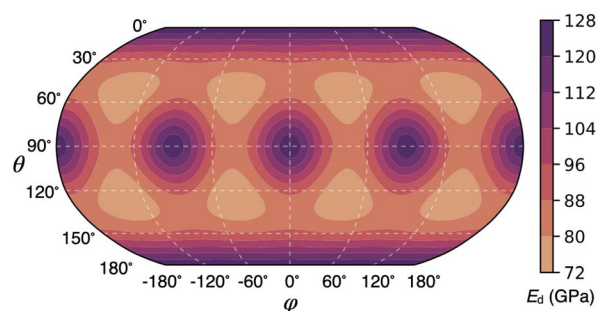


PAPERS

869

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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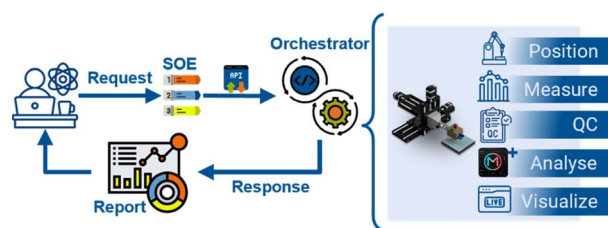


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883

Autonomous millimeter scale high throughput battery research system

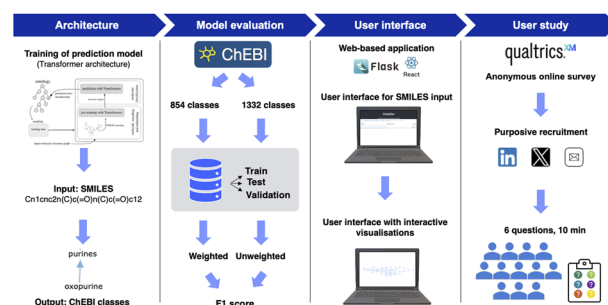
Fuzhan Rahmanian,^{*} Stefan Fuchs, Bojing Zhang, Maximilian Fichtner and Helge Sören Stein^{*}



896

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

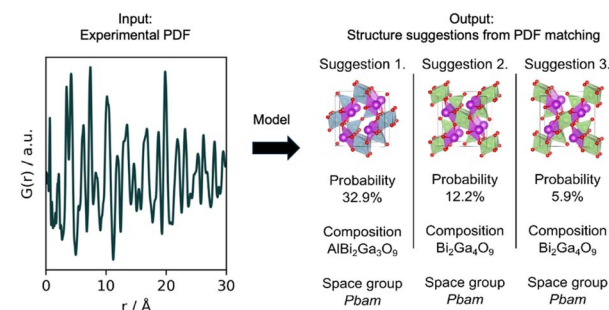
Martin Glauer, Fabian Neuhaus, Simon Flügel, Marie Wosny, Till Mossakowski, Adel Memariani, Johannes Schwerdt and Janna Hastings



908

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

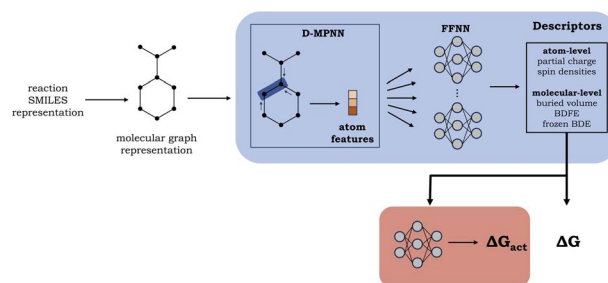
Emil T. S. Kjær, Andy S. Anker, Andrea Kirsch, Joakim Lajer, Olivia Aalling-Frederiksen, Simon J. L. Billinge^{*} and Kirsten M. Ø. Jensen^{*}



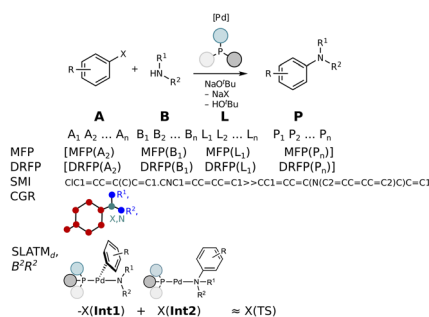
919

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^{*}



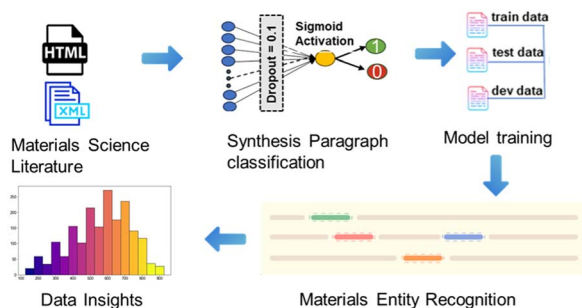
932



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*

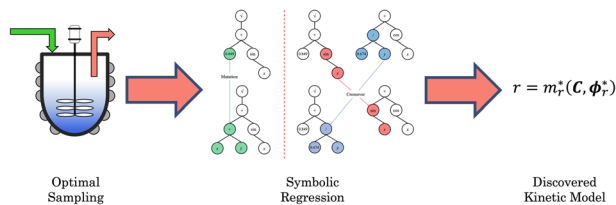
944



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

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

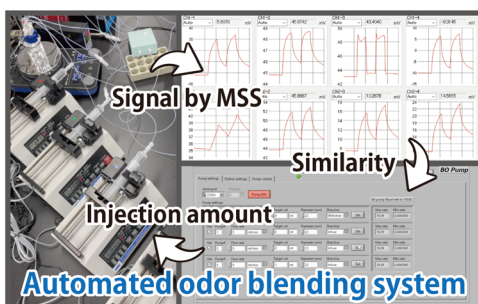
954



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*

969



Automated odor-blending with one-pot Bayesian optimization

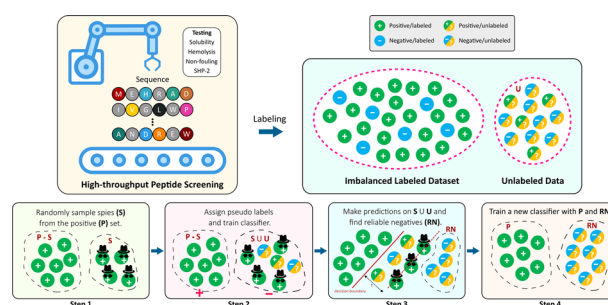
Yota Fukui, Kosuke Minami,* Kota Shiba, Genki Yoshikawa, Koji Tsuda* and Ryo Tamura*



977

Learning peptide properties with positive examples only

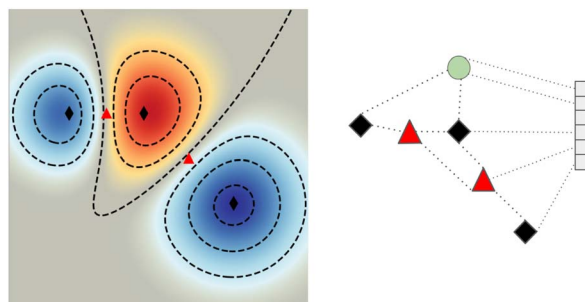
Mehrad Ansari and Andrew D. White*



987

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

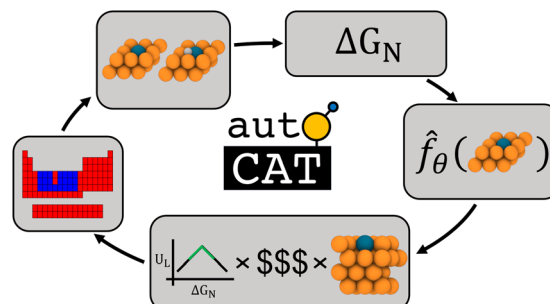
Santiago Vargas,* Winston Gee and Anastassia Alexandrova*



999

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

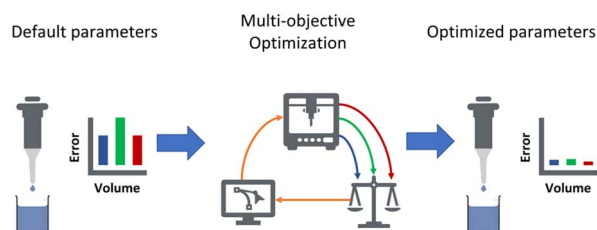
Lance Kavalsky, Vinay I. Hegde, Bryce Meredig and Venkatasubramanian Viswanathan*



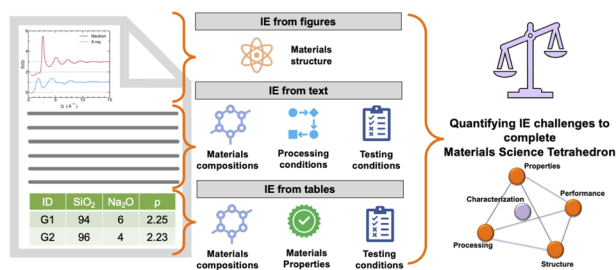
1011

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*



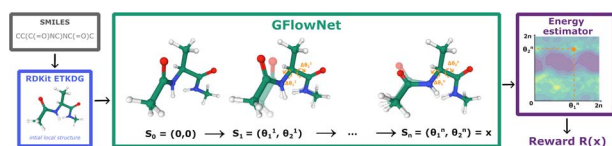
1021



Reconstructing the materials tetrahedron: challenges in materials information extraction

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

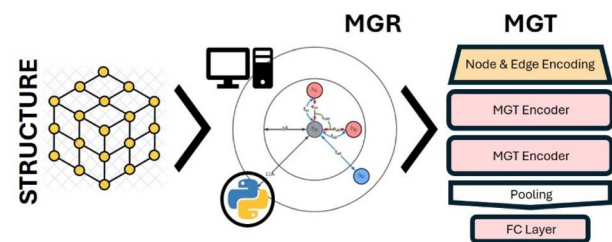
1038



Towards equilibrium molecular conformation generation with GFlowNets

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

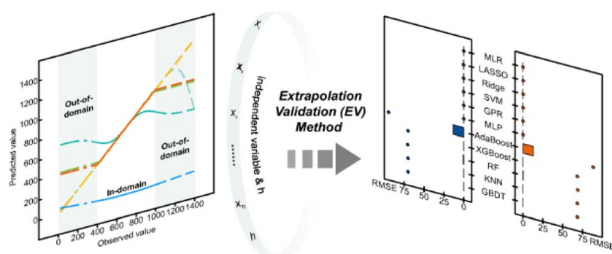
1048



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

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

1058



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

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



CORRECTIONS

1068

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*

1069

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

Mayk Caldas Ramos and Andrew D. White*

