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See Michael Nosonovsky, Ekaterina V. Skorb *et al.*, pp. 1101–1107. Image reproduced by permission of the authors from *Digital Discovery*, 2024, **3**, 1101.

Inside cover
See Francisco J. Martin-Martinez *et al.*, pp. 1108–1122. Image reproduced by permission of Francisco J. Martin-Martinez from *Digital Discovery*, 2024, **3**, 1108.

EDITORIAL

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Perspective on AI for accelerated materials design at the AI4Mat-2023 workshop at NeurIPS 2023

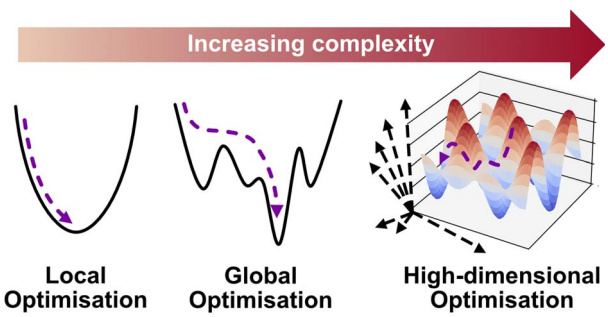
Santiago Miret,* N. M. Anoop Krishnan, Benjamin Sanchez-Lengeling, Marta Skreta, Vineeth Venugopal and Jennifer N. Wei

PERSPECTIVE

1086

Race to the bottom: Bayesian optimisation for chemical problems

Yifan Wu, Aron Walsh* and Alex M. Ganose*



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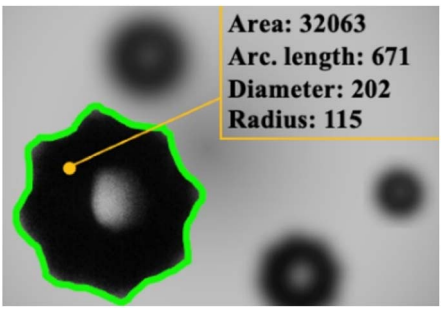
PAPERS

1101

Automatic image processing of cavitation bubbles to analyze the properties of petroleum products

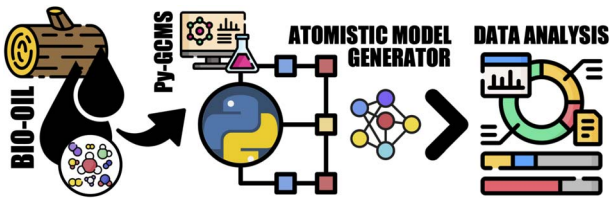
Timur Aliev, Ilya Korolev, Olga Burdulenko, Ekaterina Alchinova, Anton Subbota, Mikhail Yasnov, Michael Nosonovsky* and Ekaterina V. Skorb*



1108

Data-driven representative models to accelerate scaled-up atomistic simulations of bitumen and biobased complex fluids

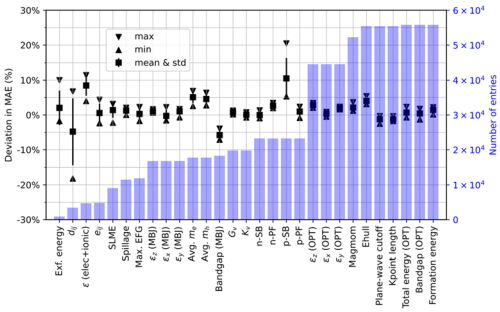
Daniel York, Isaac Vidal-Daza, Cristina Segura, Jose Norambuena-Contreras and Francisco J. Martin-Martinez*



1123

A reproducibility study of atomistic line graph neural networks for materials property prediction

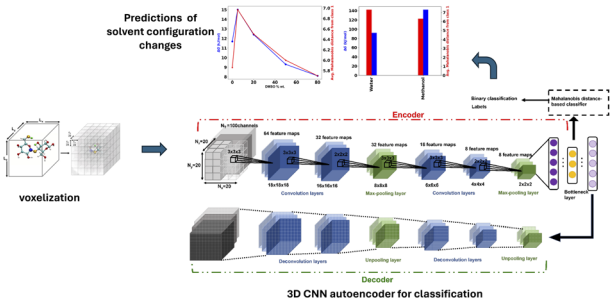
Kangming Li,* Brian DeCost, Kamal Choudhary and Jason Hattrick-Simpers



1130

A 3d convolutional neural network autoencoder for predicting solvent configuration changes in condensed phase biomass reactions

Anjana Puliyanda, Arul Mozhi Devan Padmanathan, Samir H. Mushrif and Vinay Prasad*



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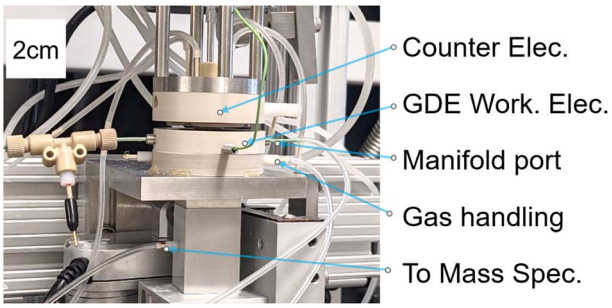
PAPERS

1144



Accelerated screening of gas diffusion electrodes for carbon dioxide reduction

Ryan J. R. Jones, Yungchieh Lai, Dan Guevarra, Kevin Kan, Joel A. Haber and John M. Gregoire*

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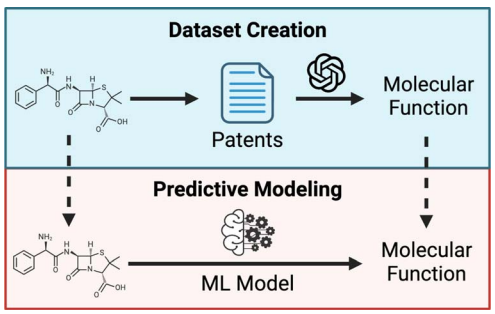

Mining patents with large language models elucidates the chemical function landscape

Clayton W. Kosonocky, Claus O. Wilke, Edward M. Marcotte and Andrew D. Ellington*

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iSIM: instant similarity

Kenneth López-Pérez, Taewon D. Kim and Ramón Alain Miranda-Quintana*

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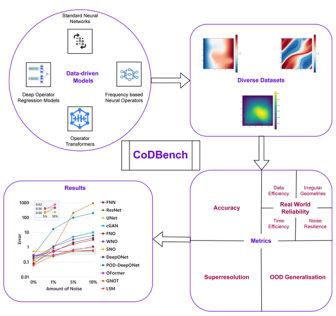

CoDBench: a critical evaluation of data-driven models for continuous dynamical systems

Priyanshu Burark, Karn Tiwari, Meer Mehran Rashid, Prathosh A. P.* and N. M. Anoop Krishnan*

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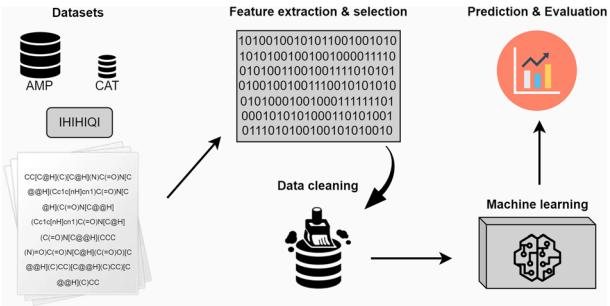
Efficiently solving the curse of feature-space dimensionality for improved peptide classification

Mario Negovetić, Erik Otović, Daniela Kalafatovic* and Goran Mauša*



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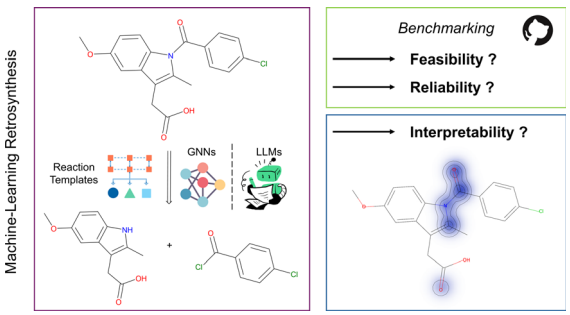
Investigating the reliability and interpretability of machine learning frameworks for chemical retrosynthesis

Friedrich Hastedt,* Rowan M. Bailey, Klaus Hellgardt, Sophia N. Yaliraki, Ehecatl Antonio del Rio Chanona* and Dongda Zhang*



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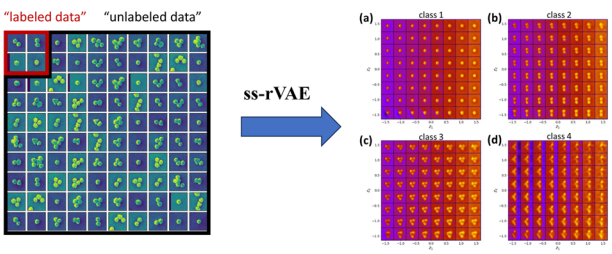
Semi-supervised learning of images with strong rotational disorder: assembling nanoparticle libraries

Maxim A. Ziatdinov,* Muammer Yusuf Yaman, Yongtao Liu, David Ginger and Sergei V. Kalinin



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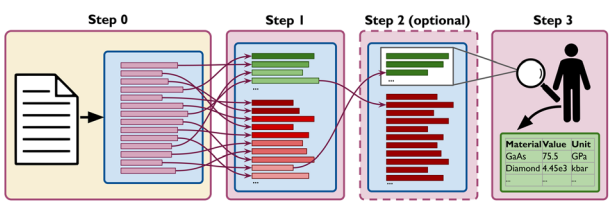
Flexible, model-agnostic method for materials data extraction from text using general purpose language models

Maciej P. Polak,* Shrey Modi, Anna Latosinska, Jinming Zhang, Ching-Wen Wang, Shaonan Wang, Ayan Deep Hazra and Dane Morgan*



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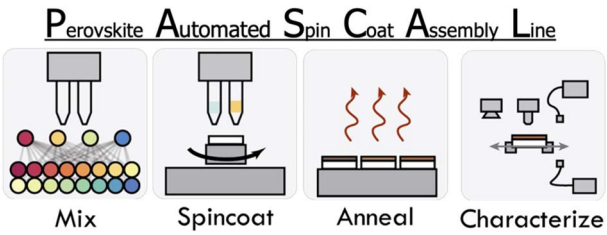

PASCAL: the perovskite automated spin coat assembly line accelerates composition screening in triple-halide perovskite alloys

Deniz N. Cakan, Rishi E. Kumar, Eric Oberholtz, Moses Kodur, Jack R. Palmer, Apoorva Gupta, Ken Kaushal, Hendrik M. Vossler and David P. Fenning*

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