

# Digital Discovery

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ISSN 2635-098X CODEN DDIIAI 3(6) 1073–1248 (2024)



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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

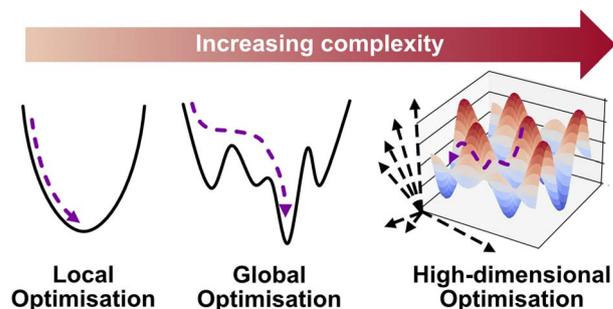


## PERSPECTIVE

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### Race to the bottom: Bayesian optimisation for chemical problems

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



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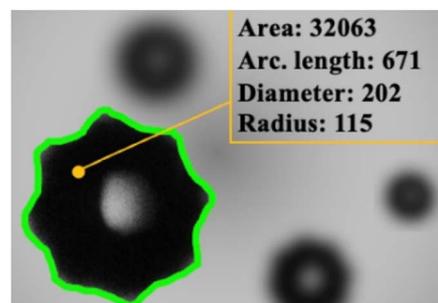
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Fundamental questions  
Elemental answers

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

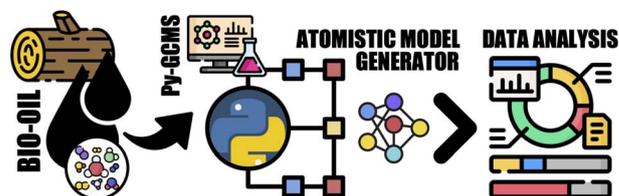
Timur Aliev, Ilya Korolev, Olga Burdulenko, Ekaterina Alchinova, Anton Subbota, Mikhail Yasnov, Michael Nosonovsky\* and Ekaterina V. Skorb\*



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

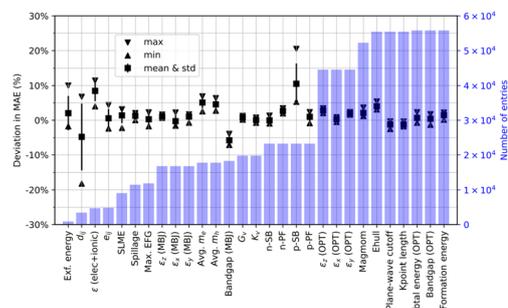
Daniel York, Isaac Vidal-Daza, Cristina Segura, Jose Norambuena-Contreras and Francisco J. Martin-Martinez\*



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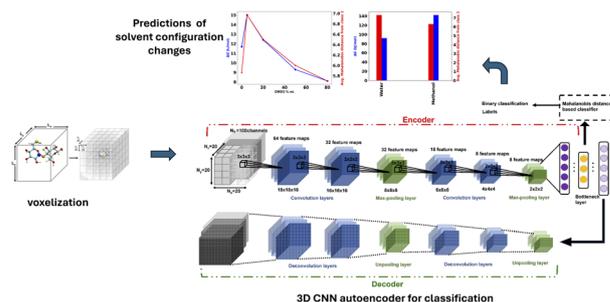
Kangming Li,\* Brian DeCost, Kamal Choudhary and Jason Hattrick-Simpers



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

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

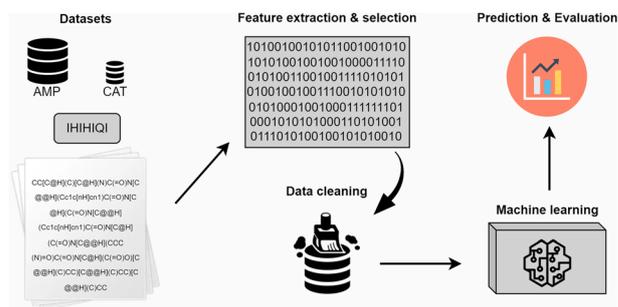




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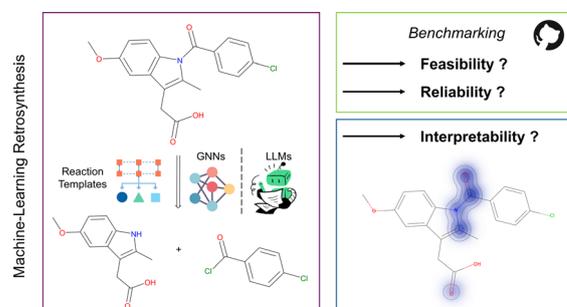
Mario Negovetić, Erik Otović, Daniela Kalafatović\* and Goran Mauša\*



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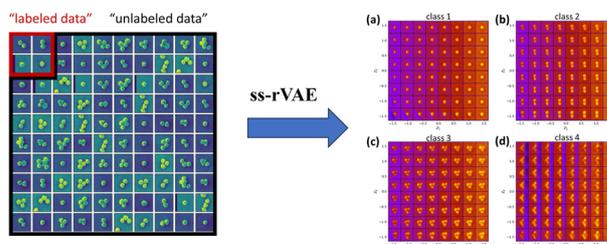
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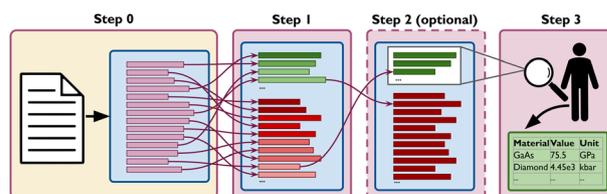
Maxim A. Ziatdinov,\* Muammer Yusuf Yaman, Yongtao Liu, David Ginger and Sergei V. Kalinin



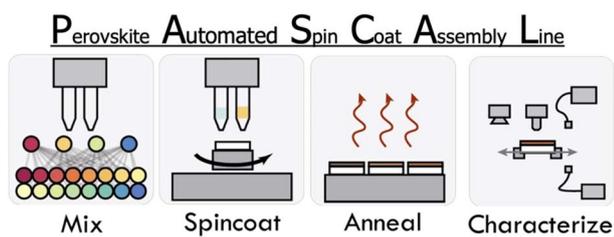
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Maciej P. Polak,\* Shrey Modi, Anna Latosinska, Jinming Zhang, Ching-Wen Wang, Shaonan Wang, Ayan Deep Hazra and Dane Morgan\*



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

