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## IN THIS ISSUE

ISSN 2635-098X CODEN DDIIAI 3(5) 833–1072 (2024)


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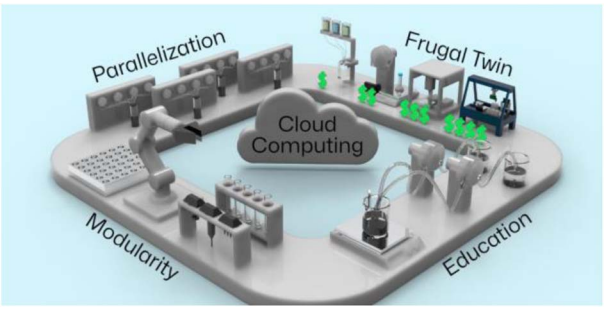
**Inside cover**
See Mingjian Wen *et al.*, pp. 869–882. Image reproduced by permission of Mingjian Wen from *Digital Discovery*, 2024, **3**, 869.

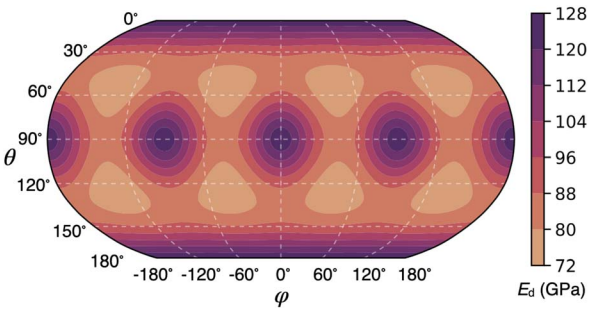
## TUTORIAL REVIEW






## PAPERS





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## PAPERS

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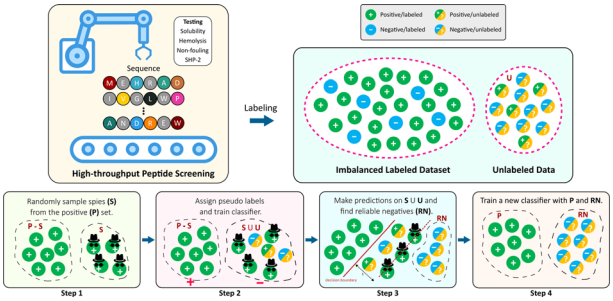
## Learning peptide properties with positive examples only

Mehrad Ansari and Andrew D. White*

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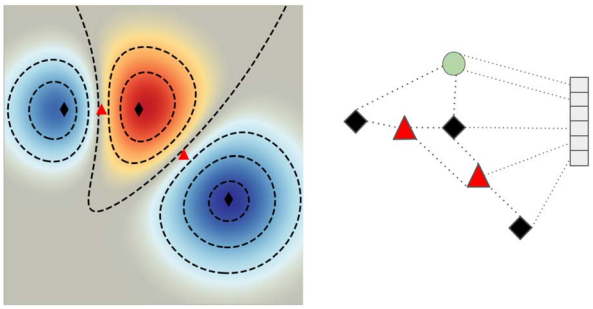
## High-throughput quantum theory of atoms in molecules (QTAIM) for geometric deep learning of molecular and reaction properties

Santiago Vargas,* Winston Gee and Anastassia Alexandrova*



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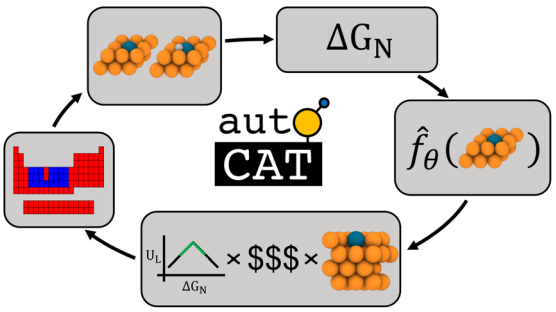
## A multiobjective closed-loop approach towards autonomous discovery of electrocatalysts for nitrogen reduction

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

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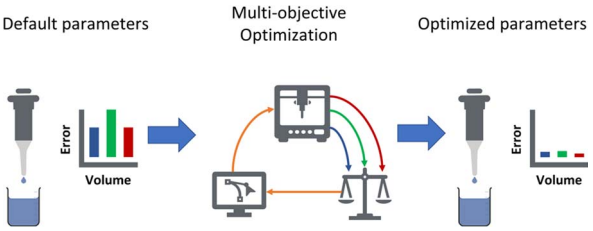
## Optimization of liquid handling parameters for viscous liquid transfers with pipetting robots, a "sticky situation"

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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## 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*