Digital Discovery

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IN THIS ISSUE

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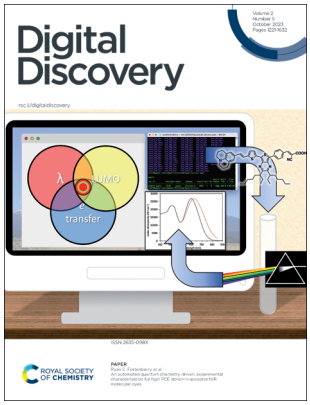

Cover
See Ryan C. Fortenberry *et al.*, pp. 1269–1288.
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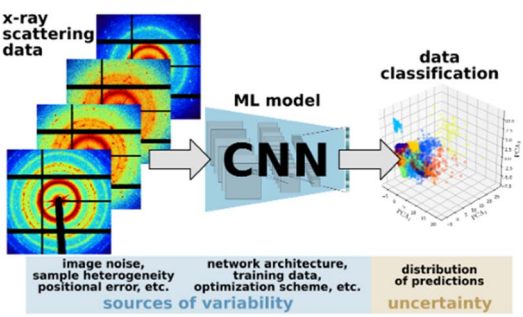
Inside cover
See Jean-Louis Reymond *et al.*, pp. 1289–1296. Image reproduced by permission of Markus Orsi from *Digital Discovery*, 2023, **2**, 1289.
Background: David Teniers the Younger, "The Alchemist". Mauritshuis, The Hague.

PERSPECTIVES



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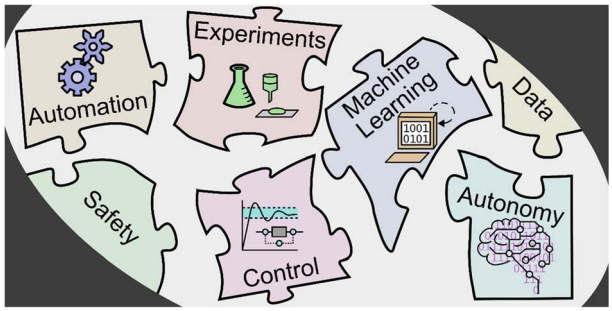

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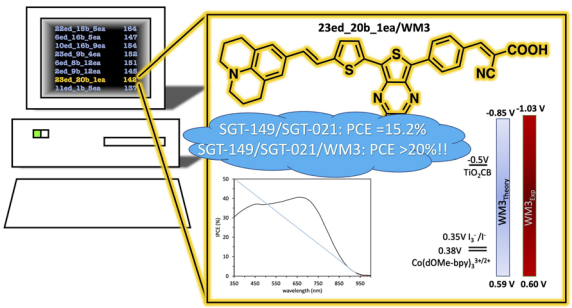

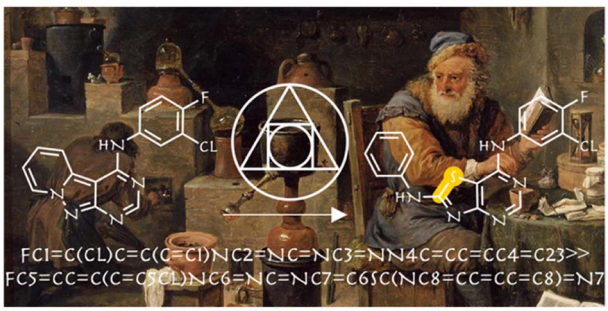

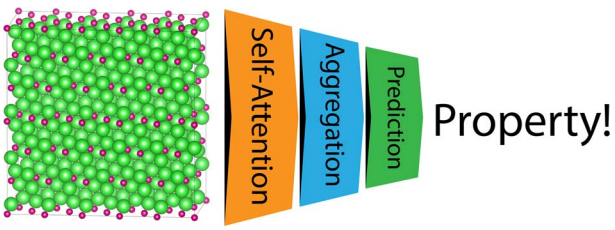

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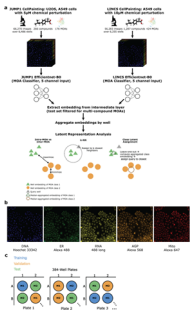

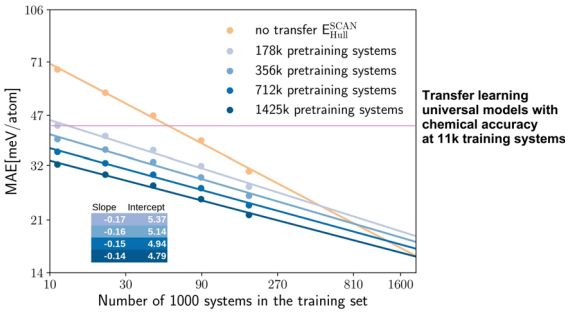

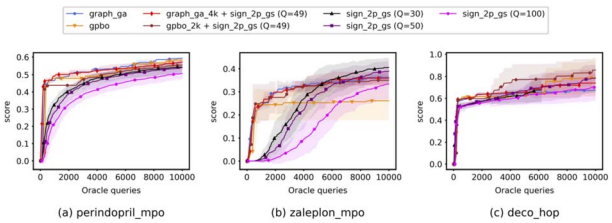

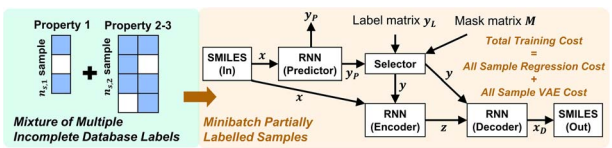

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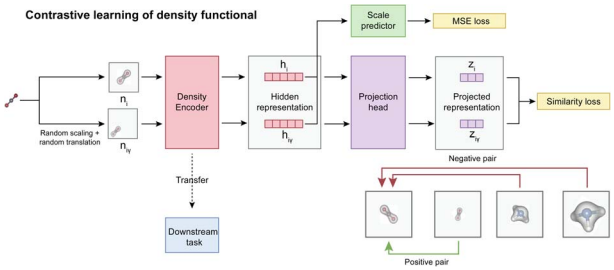

Incorporation of density scaling constraint in density functional design *via* contrastive representation learning

Weiyi Gong, Tao Sun, Hexin Bai, Shah Tanvir ur Rahman Chowdhury, Peng Chu, Anoj Aryal, Jie Yu, Haibin Ling,* John P. Perdew* and Qimin Yan*

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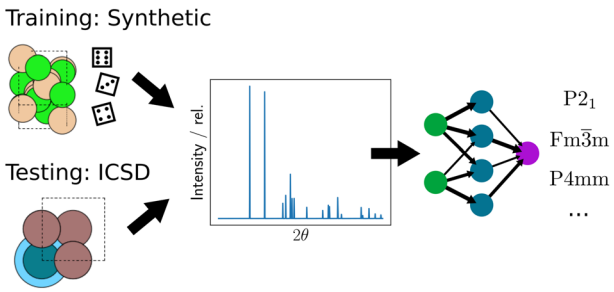

Neural networks trained on synthetically generated crystals can extract structural information from ICSD powder X-ray diffractograms

Henrik Schopmans, Patrick Reiser and Pascal Friederich*

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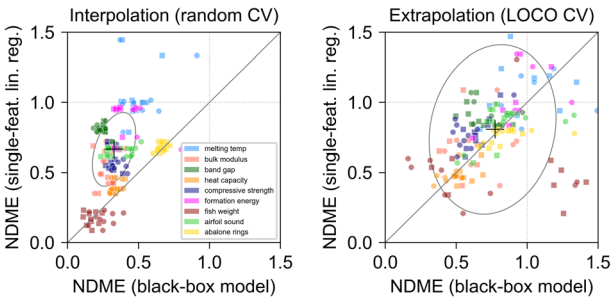

Interpretable models for extrapolation in scientific machine learning

Eric S. Muckley, James E. Saal,* Bryce Meredig, Christopher S. Roper and John H. Martin

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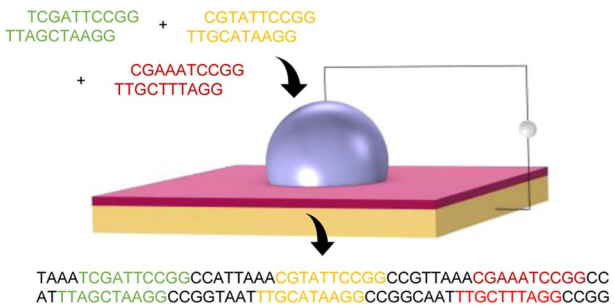

Automated routing of droplets for DNA storage on a digital microfluidics platform

Ajay Manicka, Andrew Stephan, Sriram Chari, Gemma Mendonsa, Peyton Okubo, John Stolzberg-Schray, Anil Reddy and Marc Riedel

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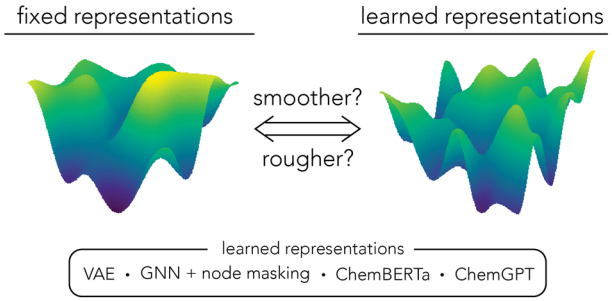
Evaluating the roughness of structure–property relationships using pretrained molecular representations

David E. Graff, Edward O. Pyzer-Knapp, Kirk E. Jordan, Eugene I. Shakhnovich and Connor W. Coley



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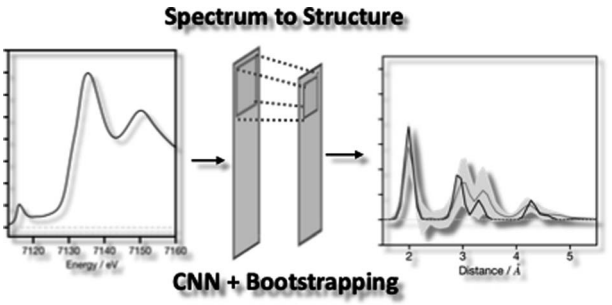
Towards the automated extraction of structural information from X-ray absorption spectra

Tudur David,* Nik Khadijah Nik Aznan, Kathryn Garside and Thomas Penfold



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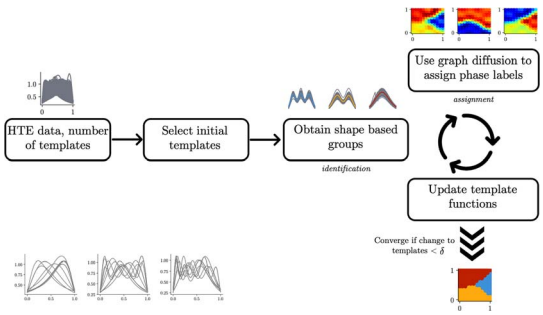
Metric geometry tools for automatic structure phase map generation

Kiran Vaddi,* Karen Li and Lilo D. Pozzo



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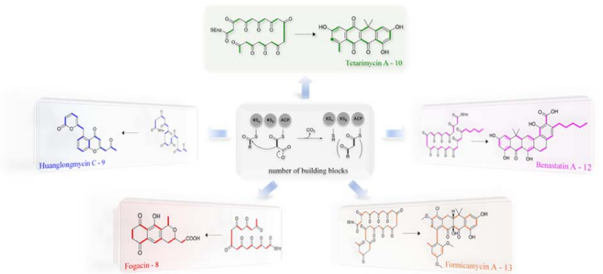
A deep learning model for type II polyketide natural product prediction without sequence alignment

Jiaquan Huang, Qiandi Gao, Ying Tang, Yaxin Wu, Heqian Zhang* and Zhiwei Qin*



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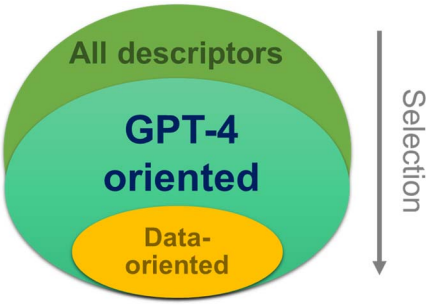

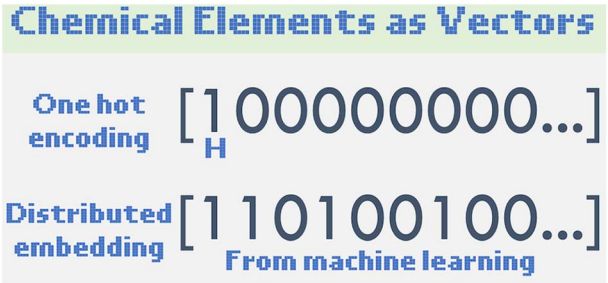

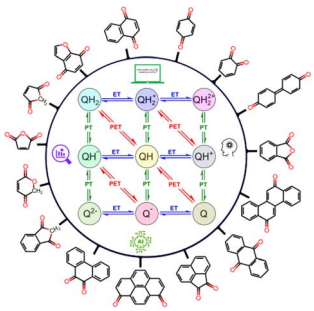

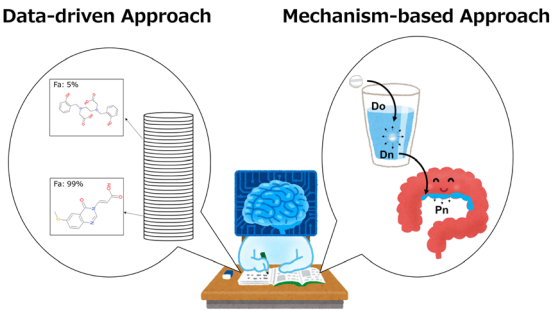

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