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See J. Pérez-Ríos *et al.*, pp. 34–50. Image reproduced by permission of Jesús Pérez-Ríos from *Digital Discovery*, 2024, **3**, 34.

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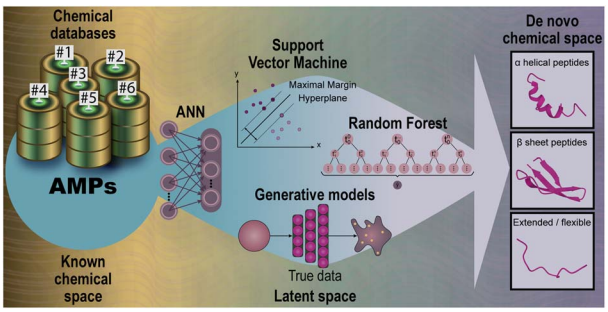

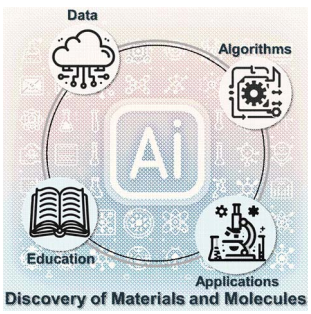

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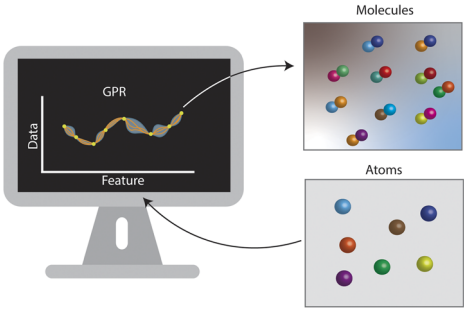
Spectroscopic constants from atomic properties: a machine learning approach

Mahmoud A. E. Ibrahim, X. Liu and J. Pérez-Ríos*



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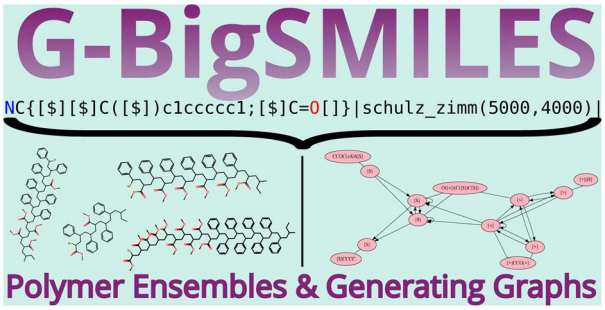
Generative BigSMILES: an extension for polymer informatics, computer simulations & ML/AI

Ludwig Schneider,* Dylan Walsh, Bradley Olsen and Juan de Pablo*



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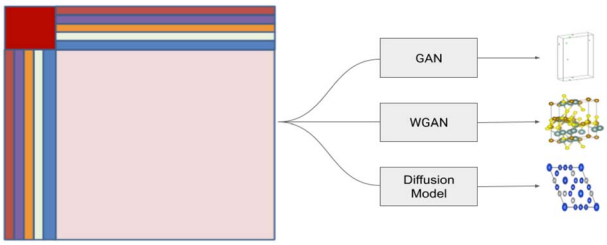
Generative adversarial networks and diffusion models in material discovery

Michael Alverson,* Sterling G. Baird, Ryan Murdock, (Enoch) Sin-Hang Ho, Jeremy Johnson and Taylor D. Sparks



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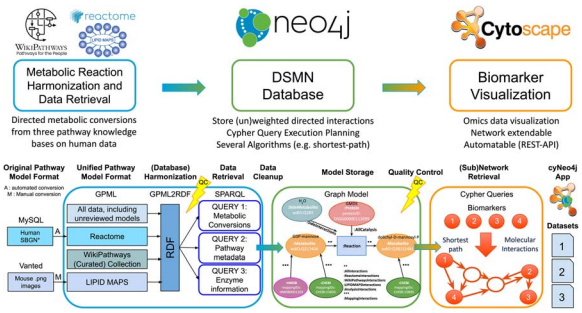
Discovering life's directed metabolic (sub)paths to interpret human biochemical markers using the DSMN tool

Denise Slenter,* Martina Kutmon, Chris T. Evelo and Egon L. Willighagen



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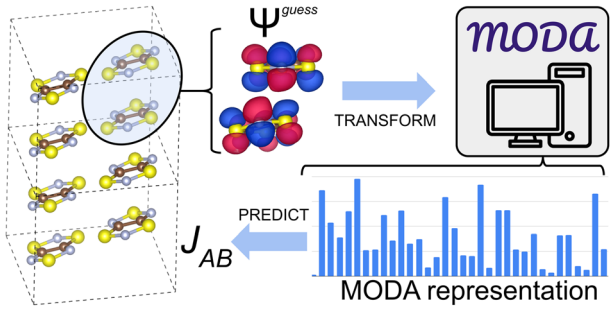

Unlocking the predictive power of quantum-inspired representations for intermolecular properties in machine learning

Raul Santiago,* Sergi Vela, Mercè Deumal and Jordi Ribas-Arino

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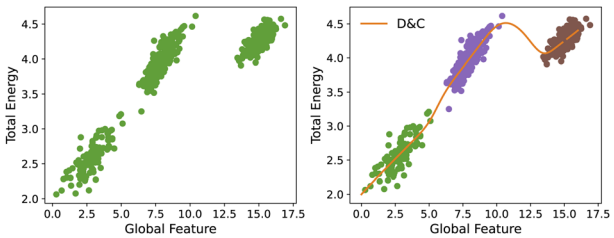

Divide-and-conquer potentials enable scalable and accurate predictions of forces and energies in atomistic systems

Claudio Zeni,* Andrea Anelli, Aldo Glielmo, Stefano de Gironcoli and Kevin Rossi*

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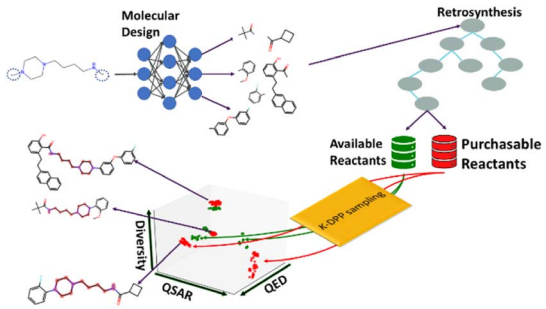

De novo generated combinatorial library design

Simon Viet Johansson,* Morteza Haghir Chehreghani, Ola Engkvist and Alexander Schliep

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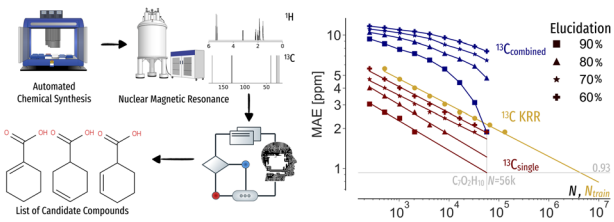

Impact of noise on inverse design: the case of NMR spectra matching

Dominik Lemm, Guido Falk von Rudorff and O. Anatole von Lilienfeld

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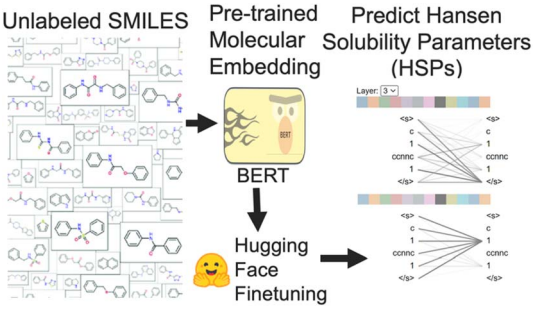

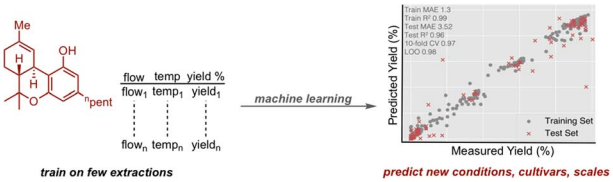

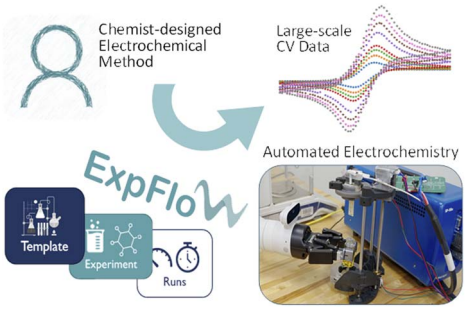

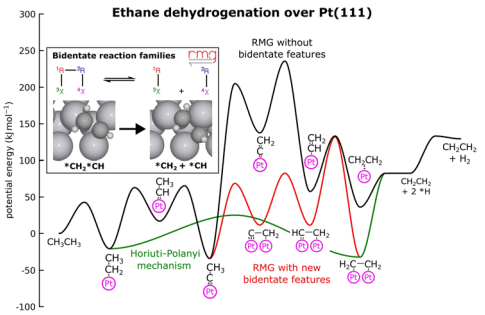

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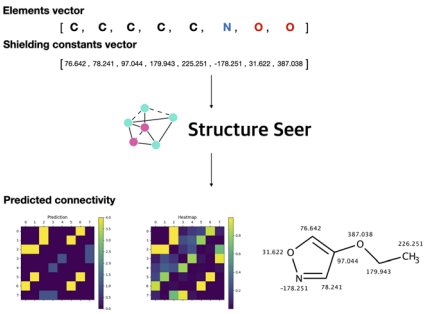

Structure Seer – a machine learning model for chemical structure elucidation from node labelling of a molecular graph

Denis Andzheevich Sapegin* and Joseph C. Bear

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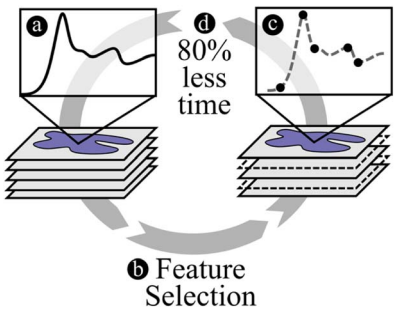

Accelerating nano-XANES imaging *via* feature selection

Samantha Tetef, Ajith Pattammattel, Yong S. Chu, Maria K. Y. Chan* and Gerald T. Seidler*

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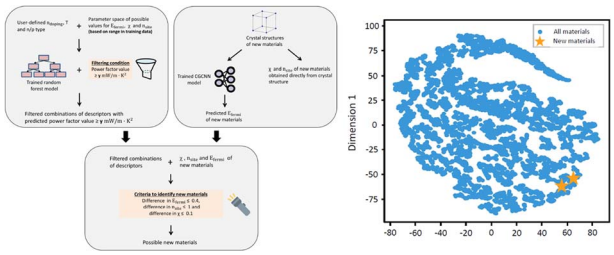

Machine learning based feature engineering for thermoelectric materials by design

U. S. Vaitesswar, Daniil Bash, Tan Huang, Jose Recatala-Gomez, Tianqi Deng, Shuo-Wang Yang, Xiaonan Wang* and Kedar Hippalgaonkar*