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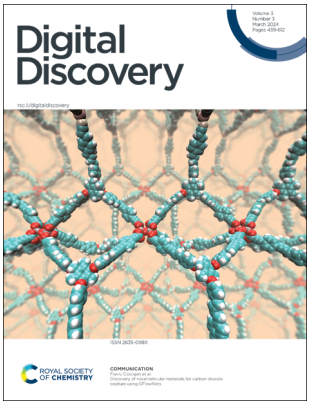

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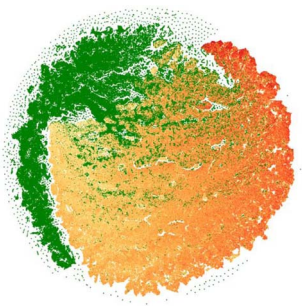

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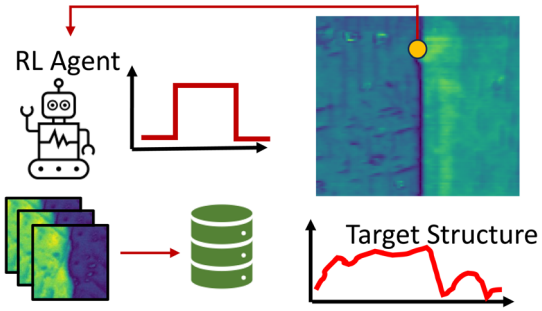
Physics-informed models of domain wall dynamics as a route for autonomous domain wall design *via* reinforcement learning

Benjamin R. Smith, Bharat Pant, Yongtao Liu, Yu-Chen Liu, Jan-Chi Yang, Stephen Jesse, Anahita Khojandi, Sergei V. Kalinin, Ye Cao and Rama K. Vasudevan*



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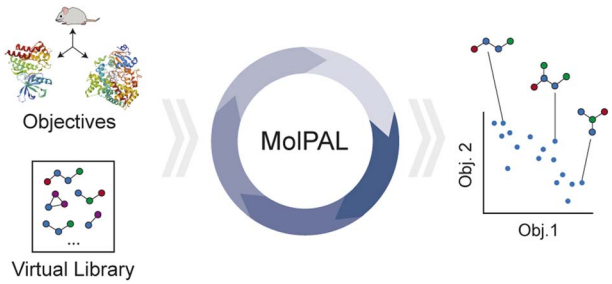

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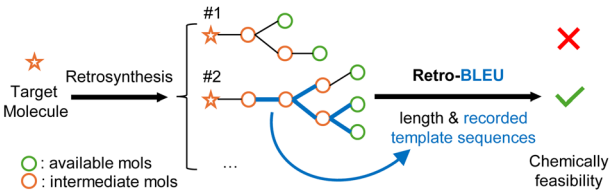
Junren Li, Lei Fang* and Jian-Guang Lou



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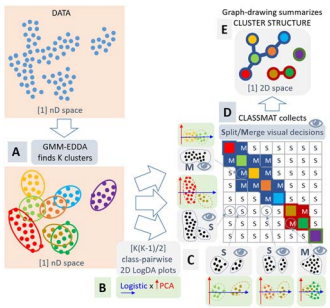

A human-in-the-loop approach for visual clustering of overlapping materials science data

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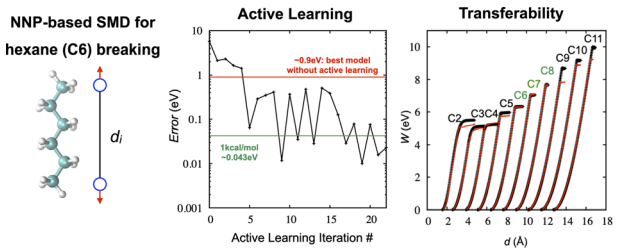

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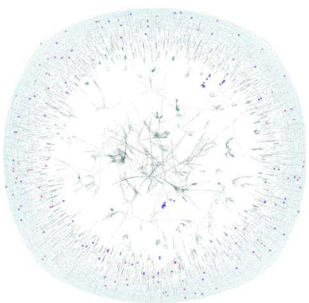

Chemical space analysis and property prediction for carbon capture solvent molecules

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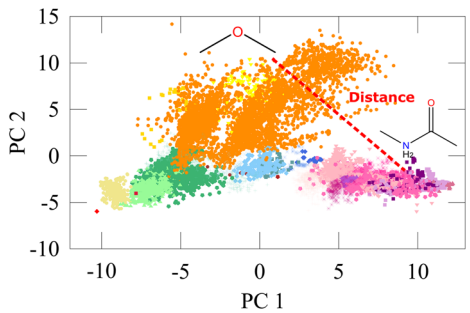

Global geometry of chemical graph neural network representations in terms of chemical moieties

Amer Marwan El-Samman,* Incé Amina Husain, Mai Huynh, Stefano De Castro, Brooke Morton and Stijn De Baerdemacker

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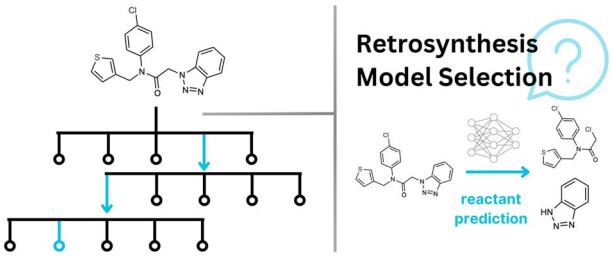
Models Matter: the impact of single-step retrosynthesis on synthesis planning

Paula Torren-Peraire,* Alan Kai Hassen,* Samuel Genheden, Jonas Verhoeven, Djork-Arné Clevert, Mike Preuss and Igor V. Tetko



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https://2DMat.ChemDX.org: Experimental data platform for 2D materials from synthesis to physical properties

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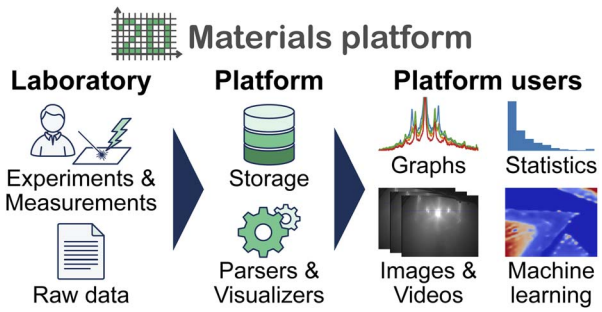

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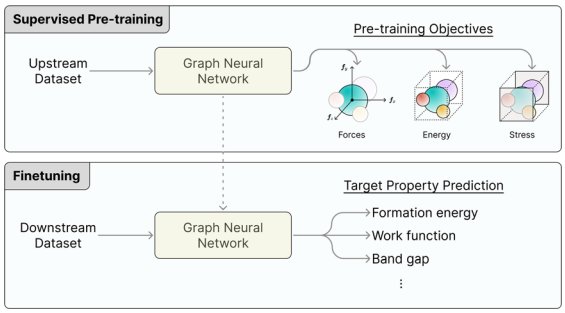
Derivative-based pre-training of graph neural networks for materials property predictions

Shuyi Jia, Akaash R. Parthasarathy, Rui Feng, Guojing Cong, Chao Zhang and Victor Fung*



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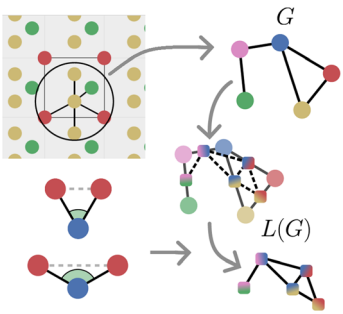
Connectivity optimized nested line graph networks for crystal structures

Robin Ruff, Patrick Reiser, Jan Stühmer and Pascal Friederich*



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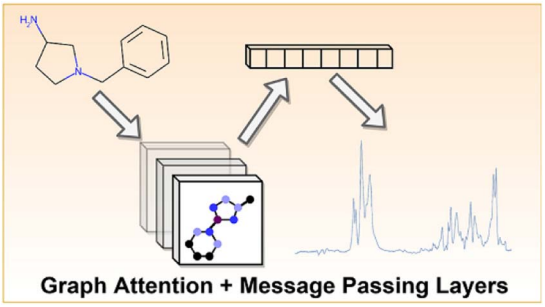

Infrared spectra prediction using attention-based graph neural networks

Naseem Saquer, Razib Iqbal,* Joshua D. Ellis and Keiichi Yoshimatsu*

CORRECTION

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Correction: Understanding the patterns that neural networks learn from chemical spectra

Laura Hannemose Rieger, Max Wilson, Tejs Vegge and Eibar Flores*

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