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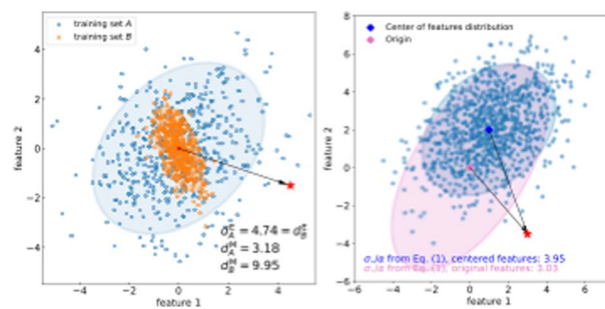
Inside cover
See Jerret Ross, Payel Das *et al.*, pp. 2684–2696. Image reproduced by permission of IBM Corporation from *Digital Discovery*, 2025, 4, 2684. Image created by Samuel Hoffman.

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Uncertainty in the era of machine learning for atomistic modeling

Federico Grasselli,* Sanggyu Chong, Venkat Kapil, Silvia Bonfanti and Kevin Rossi*

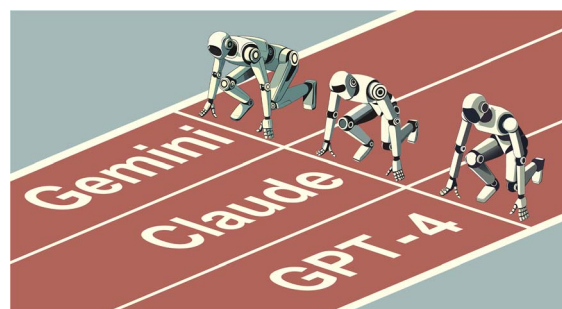


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Comparison of LLMs in extracting synthesis conditions and generating QA datasets for metal-organic frameworks

Yuang Shi, Nakul Rampal, Chengbin Zhao, Dongrong Joe Fu, Christian Borgs, Jennifer T. Chayes and Omar M. Yaghi*



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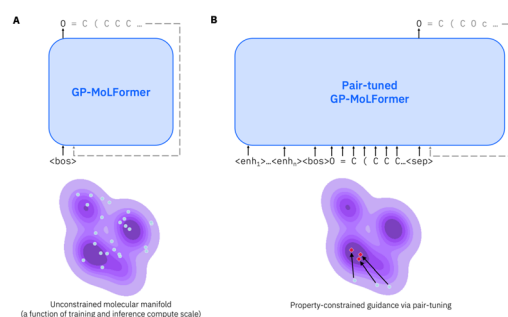
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GP-MoLFormer: a foundation model for molecular generation

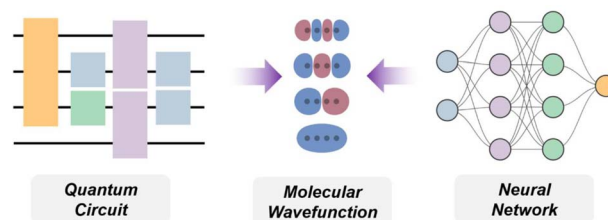
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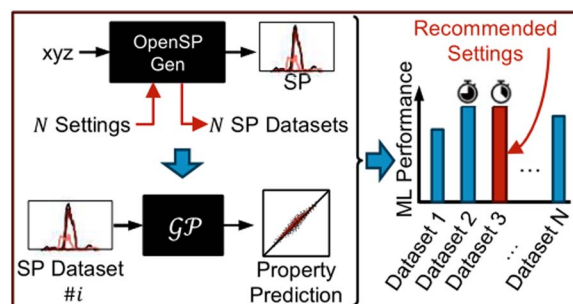
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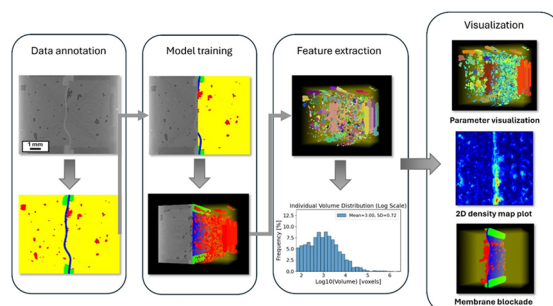
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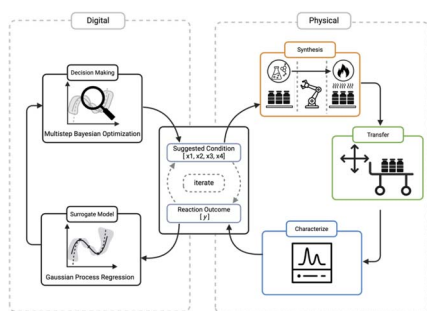
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André Colliard-Granero, Kangjun Duan, Roswitha Zeis, Michael H. Eikerling, Kourosh Malek and Mohammad J. Eslamibidgoli*



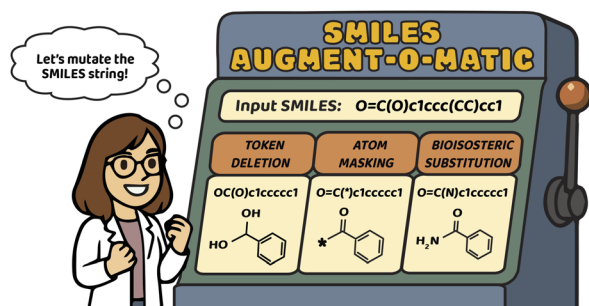
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Clara Tamura, Heather Job, Henry Chang, Wei Wang, Yangang Liang* and Shijing Sun*

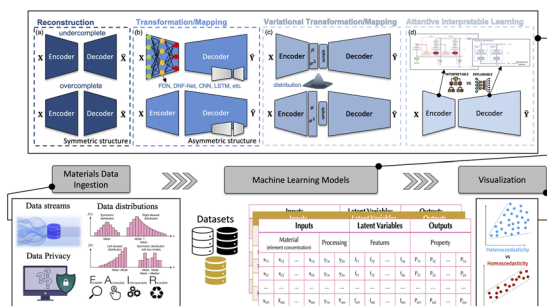
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Going beyond SMILES enumeration for data augmentation in generative drug discovery

Helena Brinkmann, Antoine Argante, Hugo ter Steege and Francesca Grisoni*

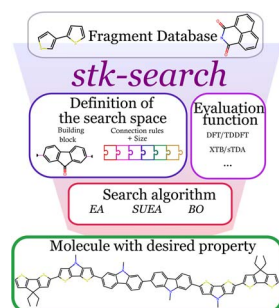
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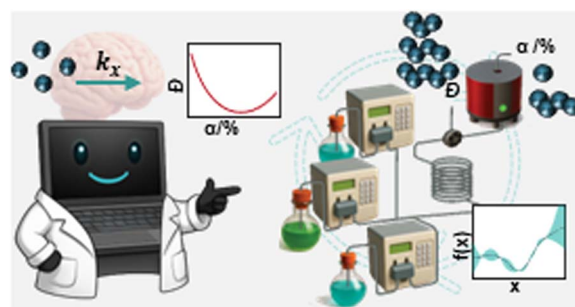
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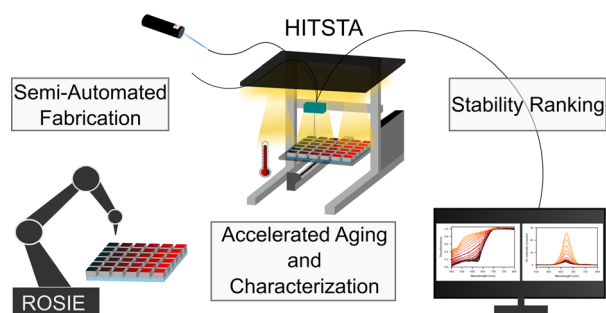
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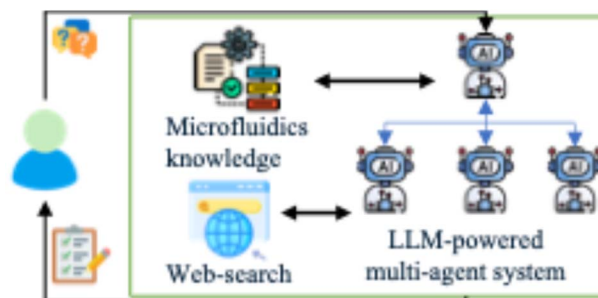
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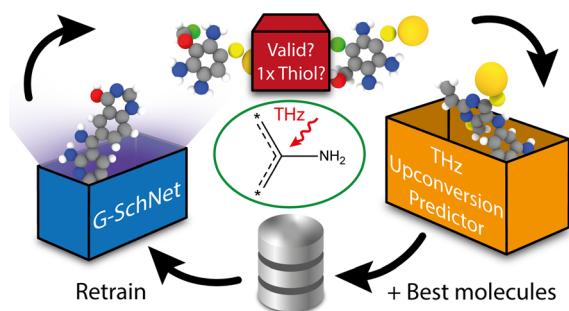
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Dinh-Nguyen Nguyen, Raymond Kai-Yu Tong and Ngoc-Duy Dinh*



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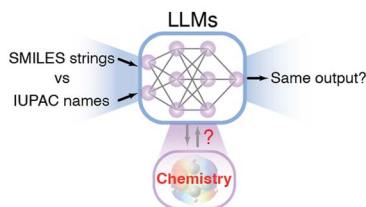


An open-source peristaltic pump with multiple independent channels for laboratory automation

Michael Buchhorn, Gun Deniz Akkoc and Dominik Dworschak*

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Do LLMs understand **chemistry** behind symbolic representations?

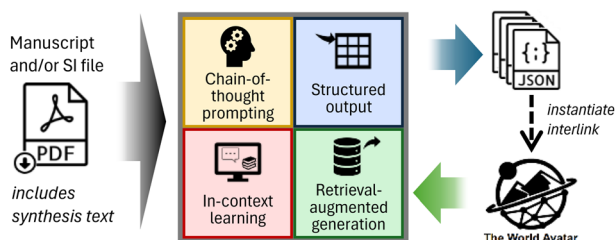


Inconsistency of LLMs in molecular representations

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Information extraction



Extraction of chemical synthesis information using the World Avatar

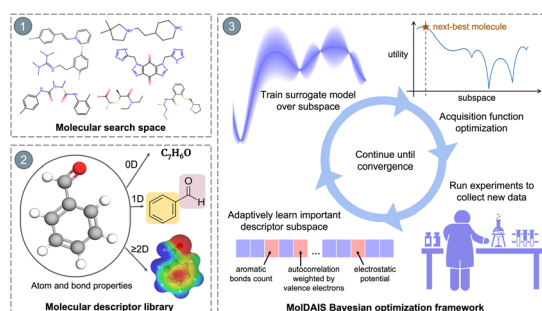
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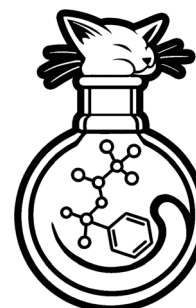
Farshud Sorourifar, Thomas Banker and Joel A. Paulson*



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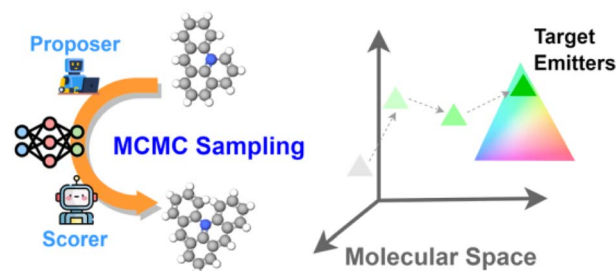
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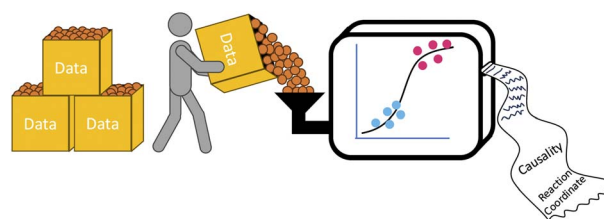
Mianzhi Pan, Tianhao Tan, Yawen Ouyang, Qian Jin, Yougang Chu, Wei-Ying Ma, Jianbing Zhang,* Lian Duan,* Dong Wang* and Hao Zhou*



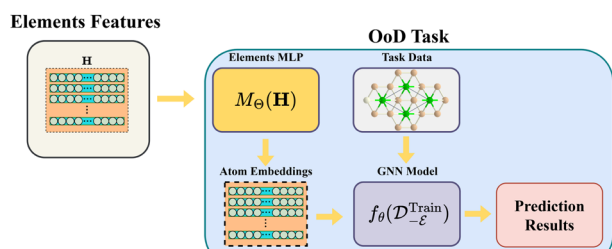
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R. A. Talmazan, J. Gamper, I. Castillo, T. S. Hofer* and M. Podewitz*



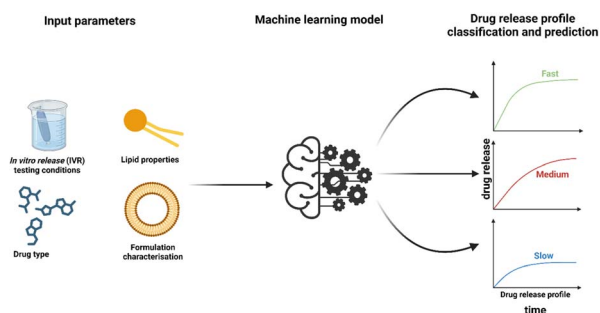
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Hamed Mahdavi,* Vasant Honavar and Dane Morgan

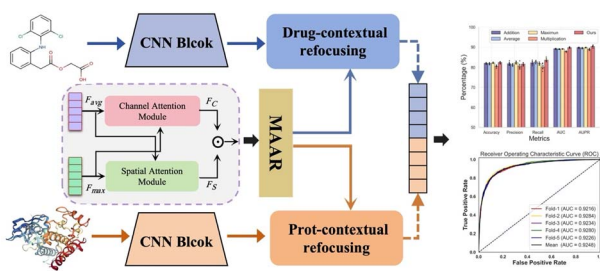
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Daniel Yanes, Vasiliki Paraskevopoulou, Heather Mead, James Mann, Magnus Röding, Maryam Parhizkar, Cameron Alexander, Jamie Twycross* and Mischa Zelzer*

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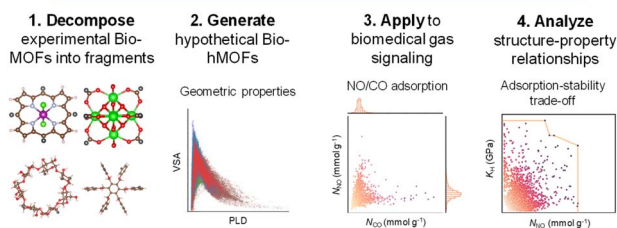


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Xinke Zhan, Tiantao Liu, Changqing Yu, Yu-An Huang, Zhuhong You and Shirley W. I. Siu*

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Digital Discovery and Design of Bio-hMOFs



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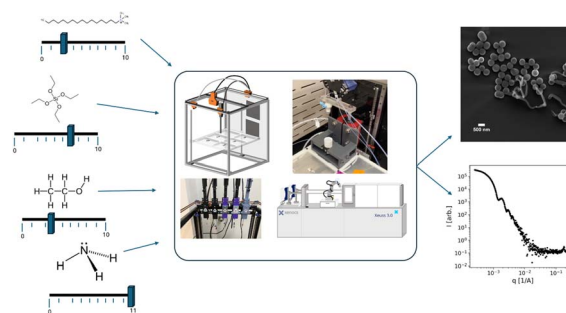
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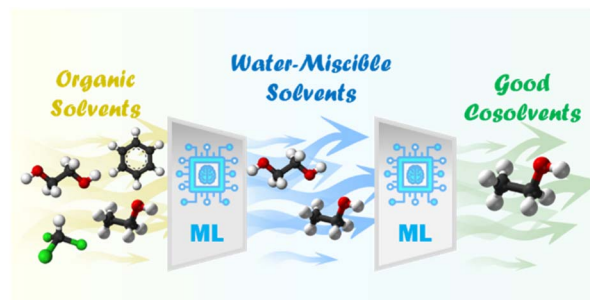
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