

Digital Discovery

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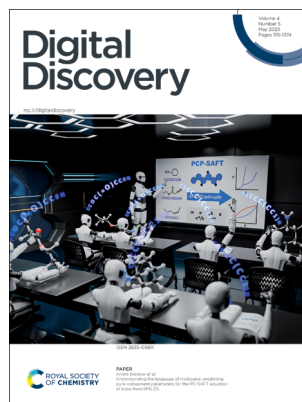
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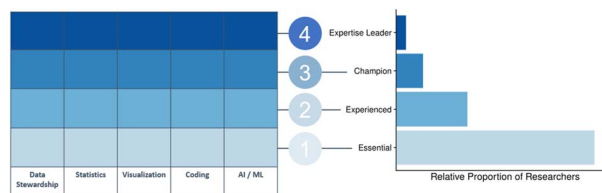
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See André Bardow *et al.*, pp. 1142–1157. Image reproduced by permission of André Bardow from *Digital Discovery*, 2025, 4, 1142. Image created by Xin Zou.

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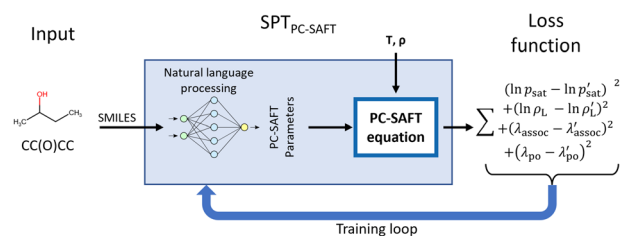
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Understanding the language of molecules: predicting pure component parameters for the PC-SAFT equation of state from SMILES

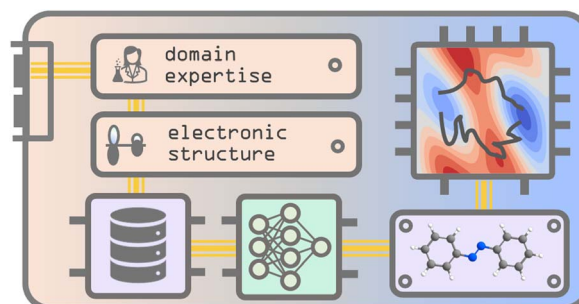
Benedikt Winter, Philipp Rehner, Timm Esper, Johannes Schilling and André Bardow*



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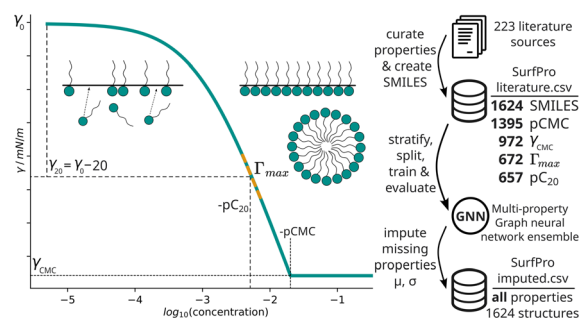
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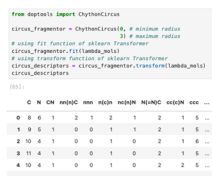
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DOPtools: a Python platform for descriptor calculation and model optimization

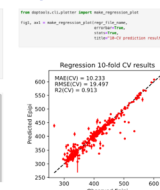
Said Byadi, Philippe Gantzer, Timur Gimadiev and Pavel Sidorov*

DOPtools

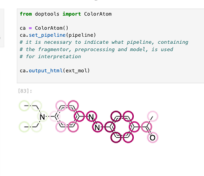
Descriptor calculation



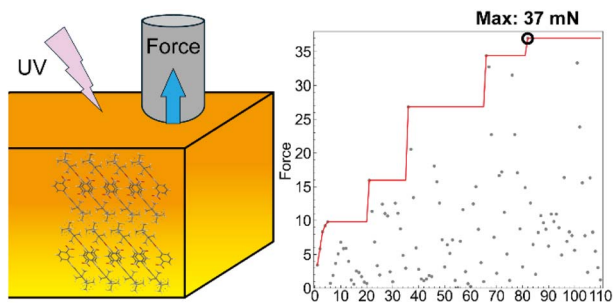
Model optimization



Model interpretation



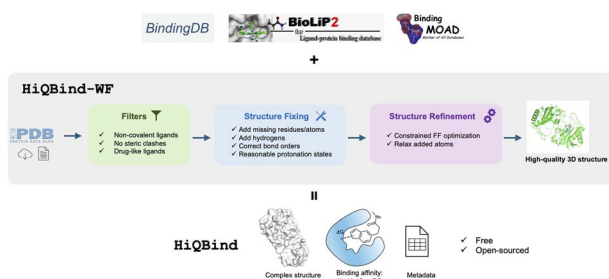
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Machine learning-driven optimization of the output force in photo-actuated organic crystals

Kazuki Ishizaki, Toru Asahi and Takuya Taniguchi*

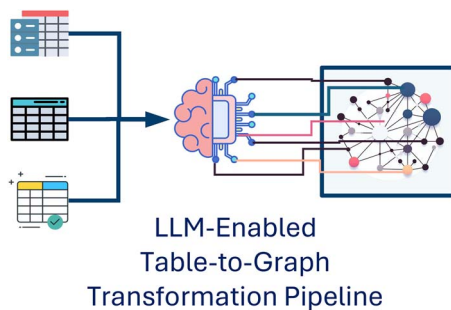
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A workflow to create a high-quality protein–ligand binding dataset for training, validation, and prediction tasks

Yingze Wang, Kunyang Sun, Jie Li, Xingyi Guan, Oufan Zhang, Dorian Bagni, Yang Zhang, Heather A. Carlson and Teresa Head-Gordon*

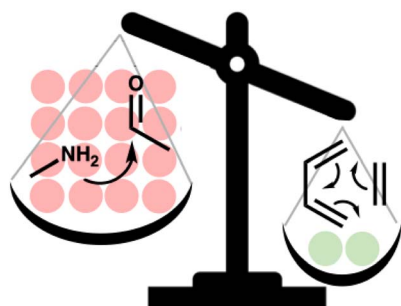
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Max Dreger,* Kourosh Malek and Michael Eikertling

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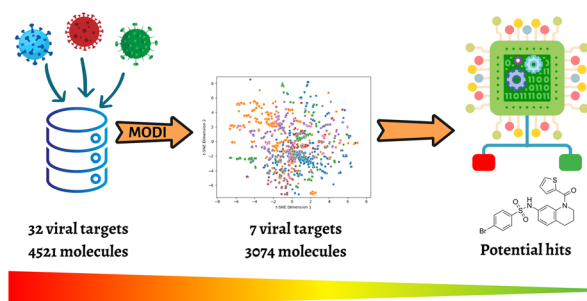
Angus Keto, Taicheng Guo, Nils Gönheimer, Xiangliang Zhang, Elizabeth H. Krenske and Olaf Wiest*



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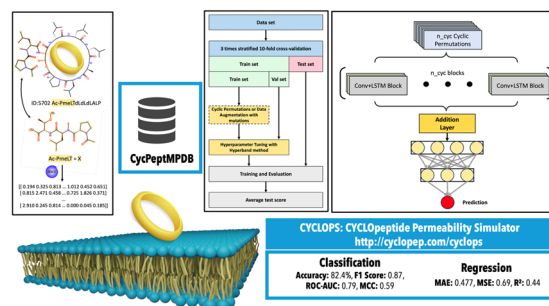
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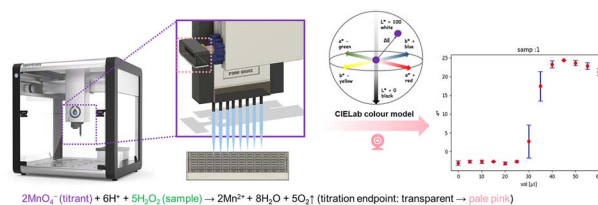
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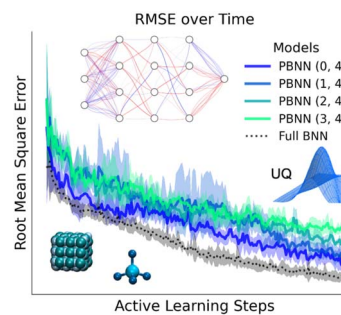
Yuan Li, Biplab Dutta, Qi Jie Yeow, Rob Clowes, Charlotte E. Boott* and Andrew I. Cooper*



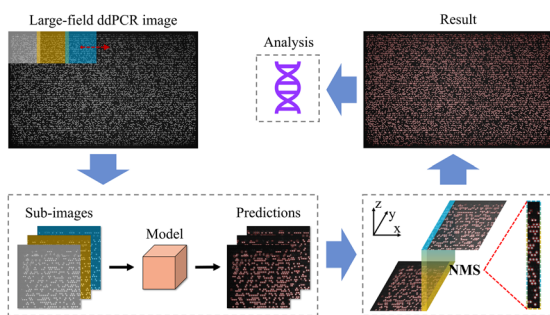
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Active and transfer learning with partially Bayesian neural networks for materials and chemicals

Sarah I. Allec and Maxim Ziatdinov*



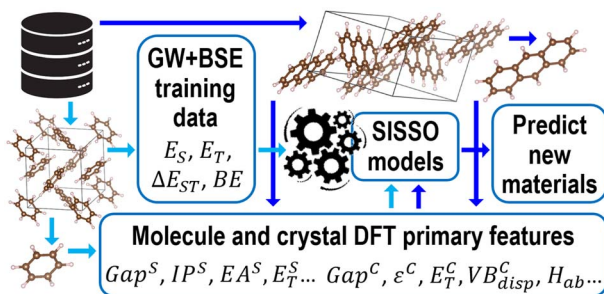
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Lightweight target detection for large-field ddPCR images based on improved YOLOv5

Xingyu Jin, Jing Yang, Xiaorui Jiang, Zhenqing Li,*
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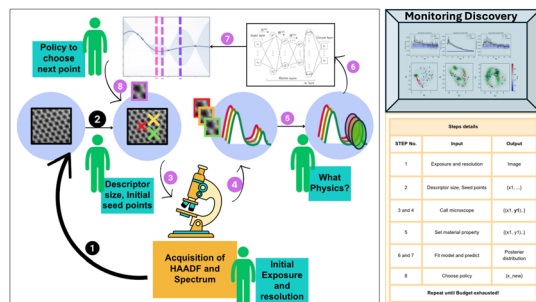
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Predicting the excited-state properties of crystalline organic semiconductors using GW+BSE and machine learning

Siyu Gao, Yiqun Luo, Xingyu Liu and Noa Marom*

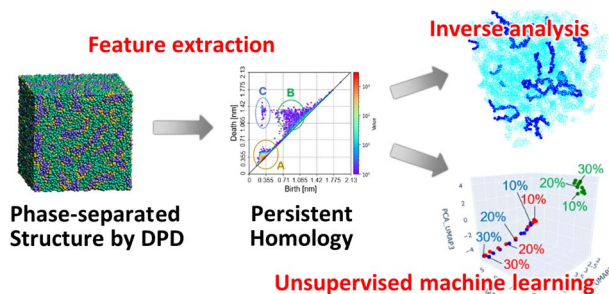
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Utkarsh Pratiush,* Kevin M. Roccapriore, Yongtao Liu,
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Feature vectorization of microphase-separated structures in polymeric materials using dissipative particle dynamics and persistent homology for machine learning applications

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