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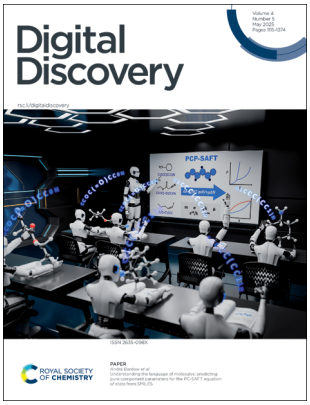

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The Citizen Data Science program at Dow

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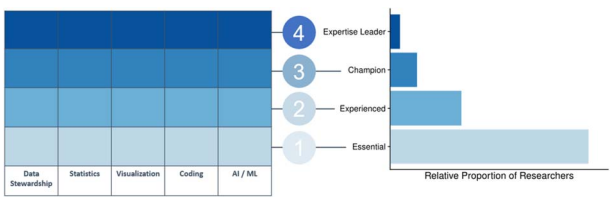

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Optimising digital twin laboratories with conversational AIs: enhancing immersive training and simulation through virtual reality

Mae V. Taylor, Zaid Muwaffak, Matthew R. Penny, Blanka R. Szulc, Steven Brown, Andy Merritt and Stephen T. Hilton*

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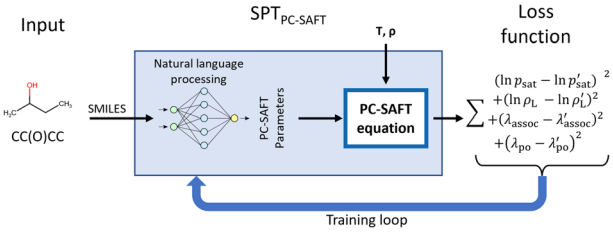
Understanding the language of molecules: predicting pure component parameters for the PC-SAFT equation of state from SMILES

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



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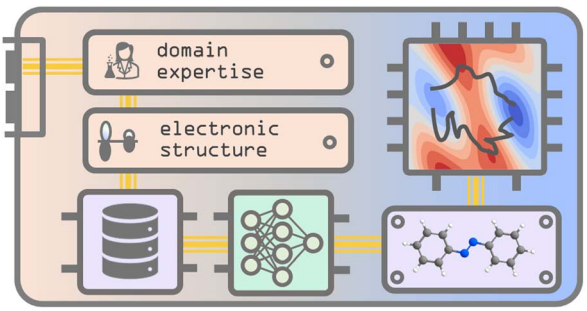
Challenges and opportunities for machine learning potentials in transition path sampling: alanine dipeptide and azobenzene studies

Nikita Fedik,* Wei Li, Nicholas Lubbers, Benjamin Nebgen, Sergei Tretiak and Ying Wai Li



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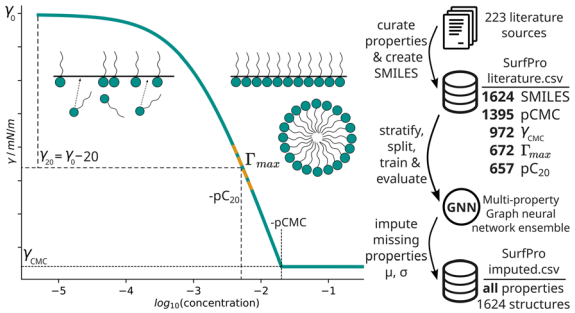
SurfPro – a curated database and predictive model of experimental properties of surfactants

Stefan L. Hödl, Luc Hermans, Pim F. J. Dankloff, Aigars Piruska, Wilhelm T. S. Huck* and William E. Robinson*



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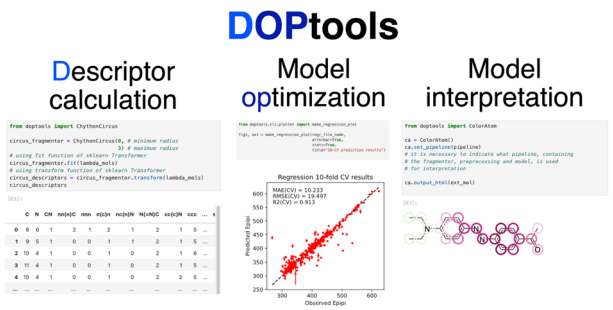
DOPtools: a Python platform for descriptor calculation and model optimization

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



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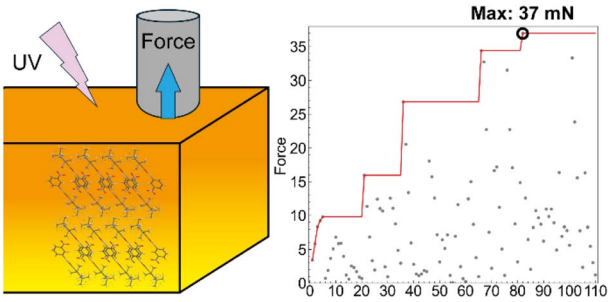

Machine learning-driven optimization of the output force in photo-actuated organic crystals

Kazuki Ishizaki, Toru Asahi and Takuya Taniguchi*

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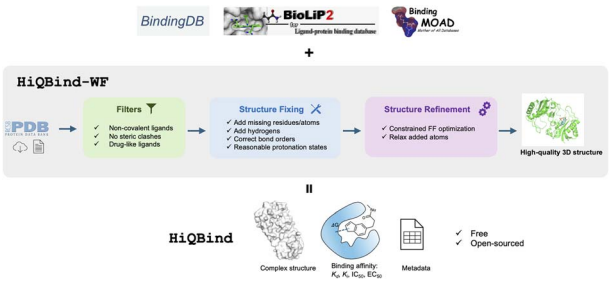

A workflow to create a high-quality protein–ligand binding dataset for training, validation, and prediction tasks

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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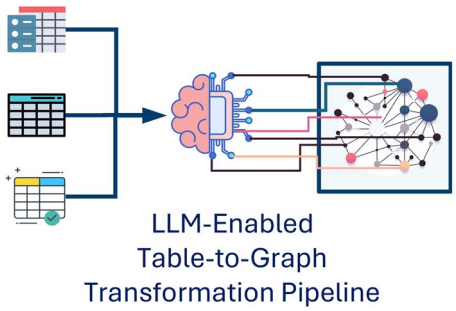

Large language models for knowledge graph extraction from tables in materials science

Max Dreger,* Kourosh Malek and Michael Eikerling

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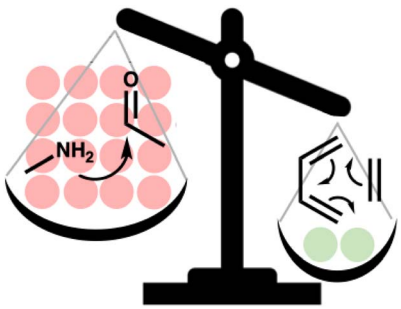

Improving reaction prediction through chemically aware transfer learning

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

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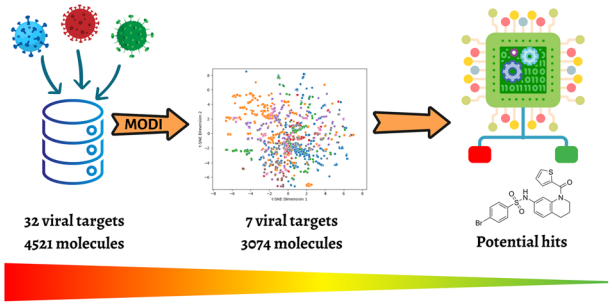
Machine learning-driven antiviral libraries targeting respiratory viruses

Gabriela Valle-Núñez, Raziel Cedillo-González, Juan F. Avellaneda-Tamayo, Fernanda I. Saldívar-González, Diana L. Prado-Romero and José L. Medina-Franco*



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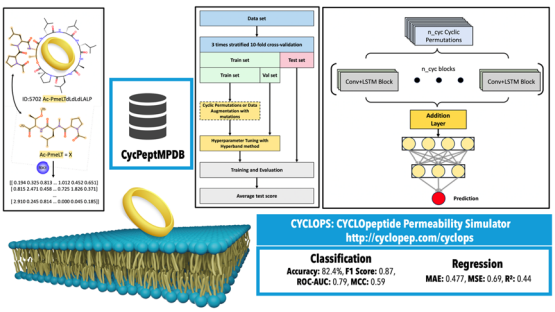
Unravelling cyclic peptide membrane permeability prediction: a study on data augmentation, architecture choices, and representation schemes

Alfonso Cabezón, Erik Otović, Daniela Kalafatovic, Ángel Piñeiro, Rebeca García-Fandiño* and Goran Mauša*



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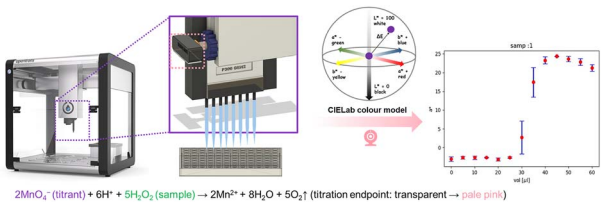
High-throughput robotic colourimetric titrations using computer vision

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



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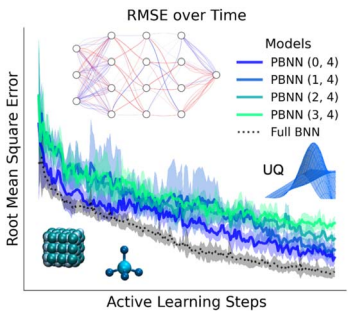
Active and transfer learning with partially Bayesian neural networks for materials and chemicals

Sarah I. Allec and Maxim Ziatdinov*



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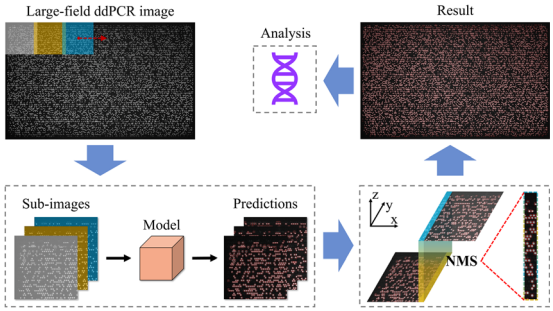

Lightweight target detection for large-field ddPCR images based on improved YOLOv5

Xingyu Jin, Jing Yang, Xiaorui Jiang, Zhenqing Li,* Jinrong Shen, Zhiheng Yu, Cunliang Yang, Fengli Huang, Dunlu Peng, Yoshinori Yamaguchi and Jijun Feng*

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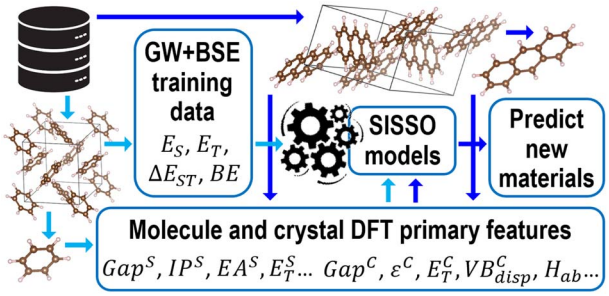

Predicting the excited-state properties of crystalline organic semiconductors using GW+BSE and machine learning

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

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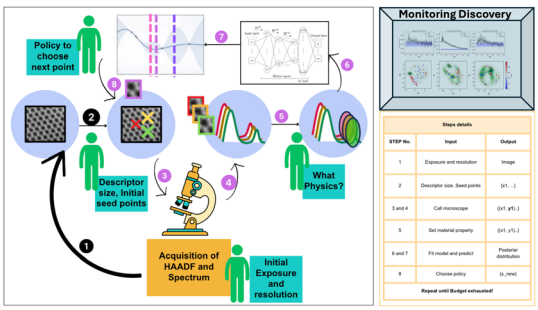

Building workflows for an interactive human-in-the-loop automated experiment (hAE) in STEM-EELS

Utkarsh Pratiush,* Kevin M. Roccapriore, Yongtao Liu, Gerd Duscher, Maxim Ziatdinov and Sergei V. Kalinin*

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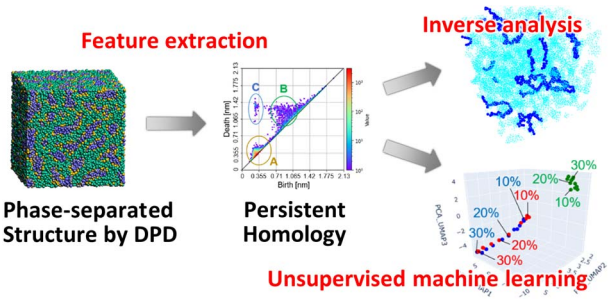

Feature vectorization of microphase-separated structures in polymeric materials using dissipative particle dynamics and persistent homology for machine learning applications

Yukito Higashi, Koji Okuwaki, Yuji Mochizuki, Tsuyohiko Fujigaya* and Koichiro Kato*

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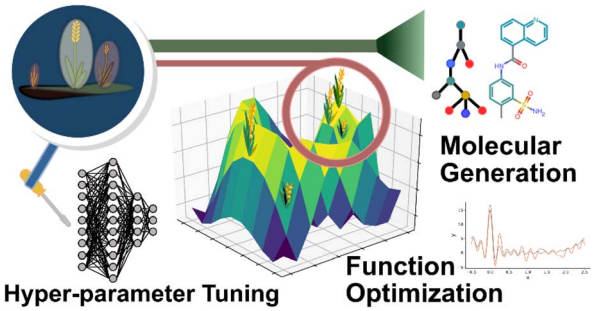
Paddy: an evolutionary optimization algorithm for chemical systems and spaces

Armen G. Beck, Sanjay Iyer, Jonathan Fine and Gaurav Chopra*



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