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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.

PERSPECTIVE

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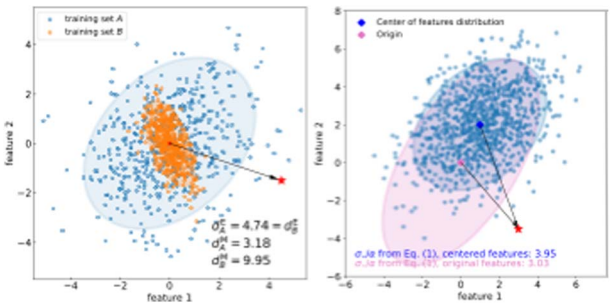
Uncertainty in the era of machine learning for atomistic modeling

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



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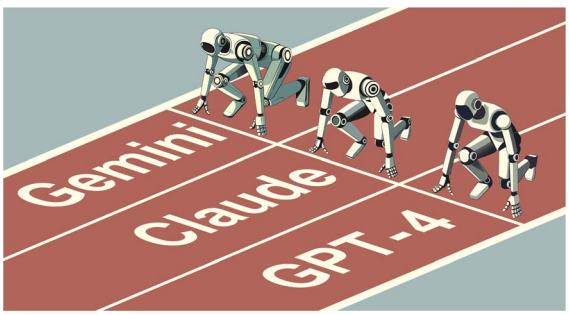
Comparison of LLMs in extracting synthesis conditions and generating QA datasets for metal–organic frameworks

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



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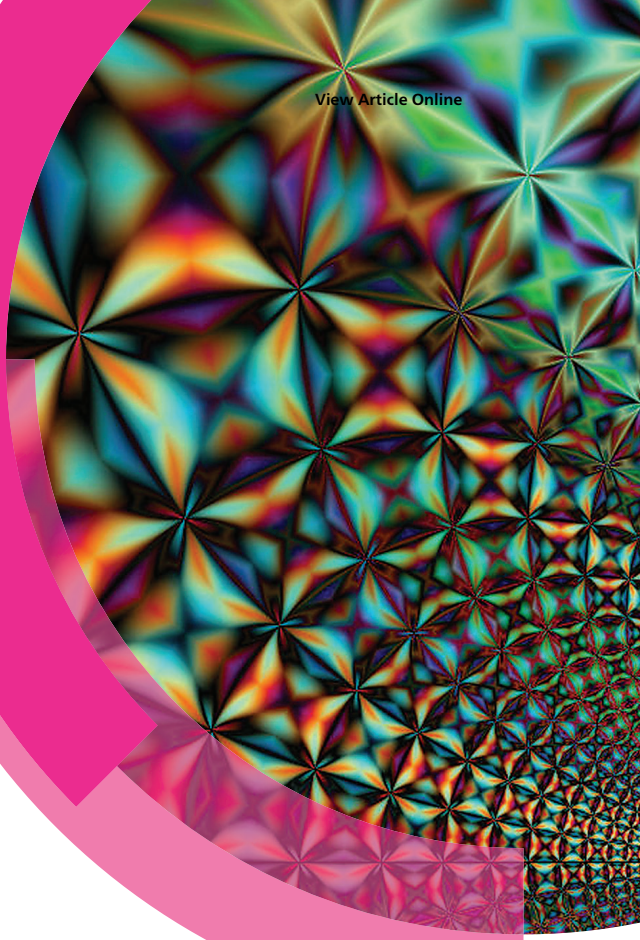

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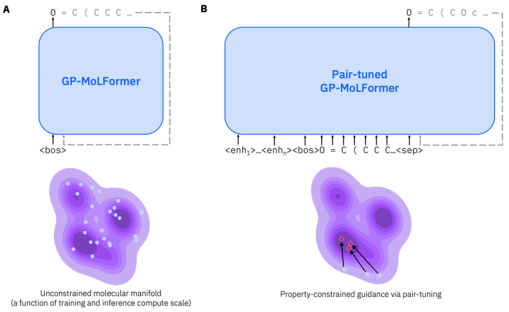
GP-MoLFormer: a foundation model for molecular generation

Jerret Ross,* Brian Belgodere, Samuel C. Hoffman, Vijil Chenthamarakshan, Jiri Navratil, Youssef Mroueh and Payel Das*



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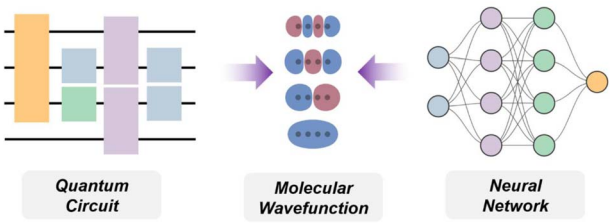
Quantum machine learning of molecular energies with hybrid quantum-neural wavefunction

Weitang Li,* Shi-Xin Zhang, Zirui Sheng, Cunxi Gong, Jianpeng Chen and Zhigang Shuai



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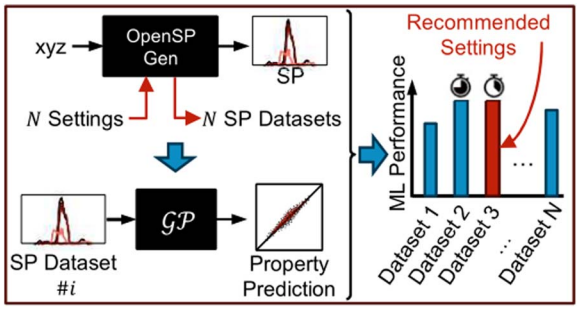
Open-source generation of sigma profiles: impact of quantum chemistry and solvation treatment on machine learning performance

Fathya Y. M. Salih, Dinis O. Abranches, Edward J. Maginn and Yamil J. Colón*



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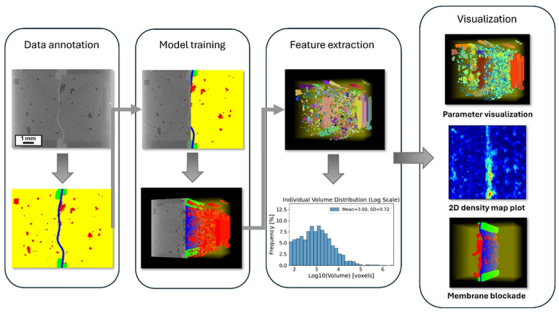
Advancing vanadium redox flow battery analysis: a deep learning approach for high-throughput 3D visualization and bubble quantification

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



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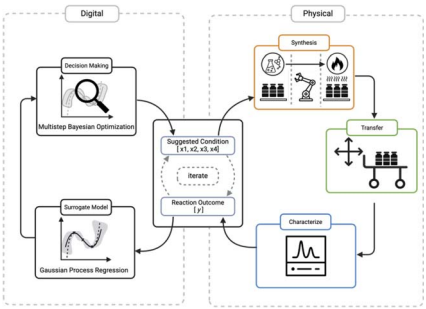

Autonomous organic synthesis for redox flow batteries *via* flexible batch Bayesian optimization

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

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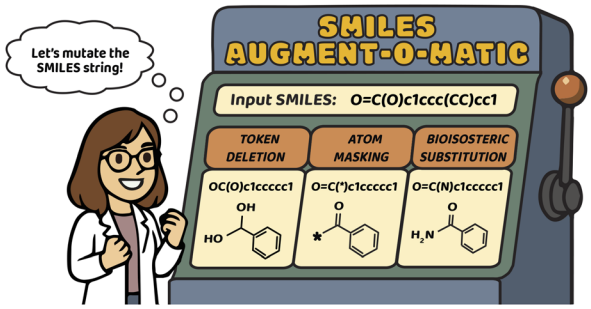

Going beyond SMILES enumeration for data augmentation in generative drug discovery

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

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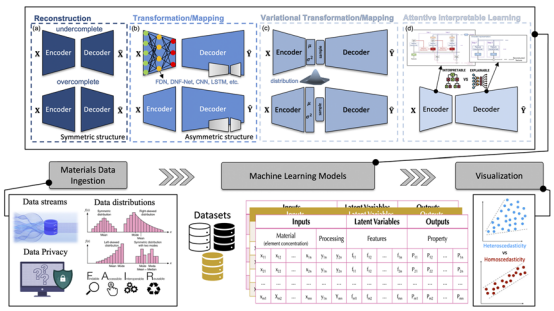

Decoding non-linearity and complexity: deep tabular learning approaches for materials science

Vahid Attari* and Raymundo Arroyave

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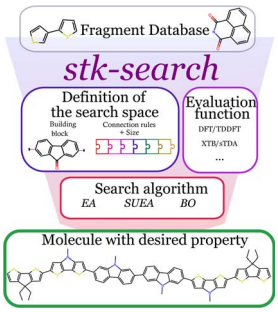

Comparative analysis of search approaches to discover donor molecules for organic solar cells

Mohammed Azzouzi,* Steven Bennett, Victor Posligua, Roberto Bondesan, Martijn A. Zwijnenburg and Kim E. Jelfs*

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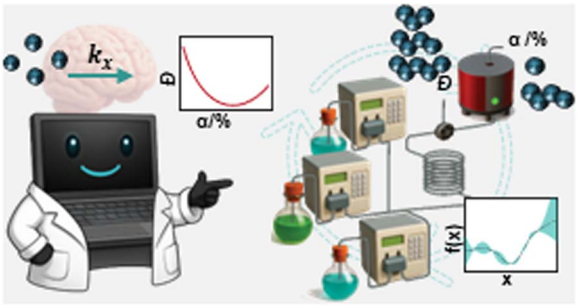
Integrating mechanistic modelling with Bayesian optimisation: accelerated self-driving laboratories for RAFT polymerisation

Clarissa. Y. P. Wilding,* Richard. A. Bourne and Nicholas. J. Warren*



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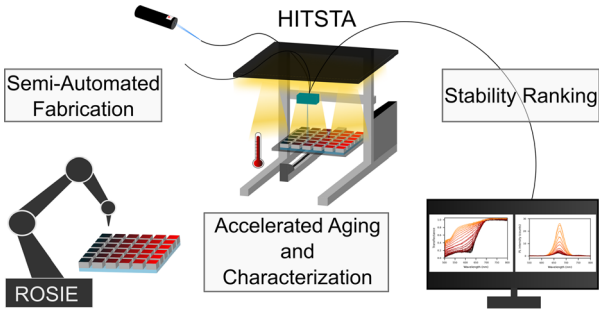
Accelerating optimization of halide perovskites: two blueprints for automation

Hilal Aybike Can,* Daniel Anthony Jacobs, Nicolas Fürst, Christophe Ballif and Christian Michael Wolff*



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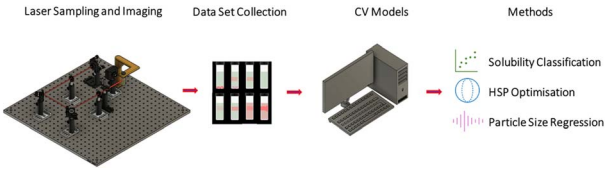
Computer vision for polymer characterisation using lasers

Seda Uyanik, Sam Parkinson, George Killick, Biplab Dutta, Rob Clowes, Charlotte E. Boott* and Andrew I. Cooper*



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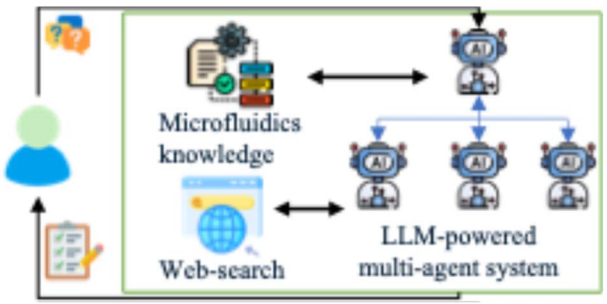
DropMicroFluidAgents (DMFAs): autonomous droplet microfluidic research framework through large language model agents

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



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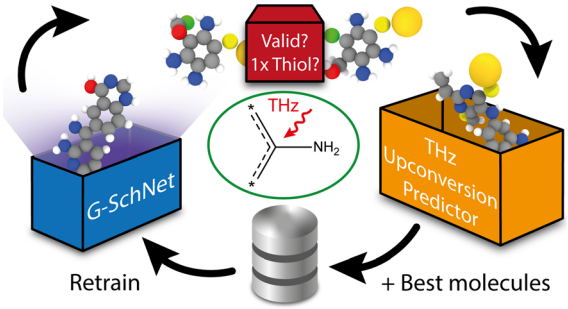

Generative design of functional organic molecules for terahertz radiation detection

Zsuzsanna Koczor-Benda,* Shayantan Chaudhuri, Joe Gilkes, Francesco Bartucca, Liming Li and Reinhard J. Maurer*

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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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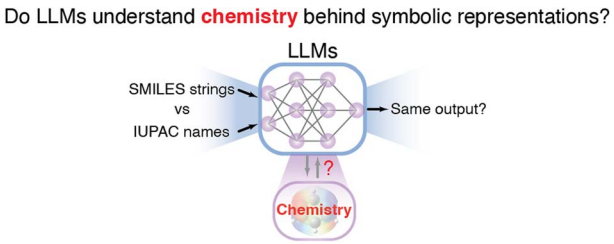

Inconsistency of LLMs in molecular representations

Bing Yan, Angelica Chen and Kyunghyun Cho*

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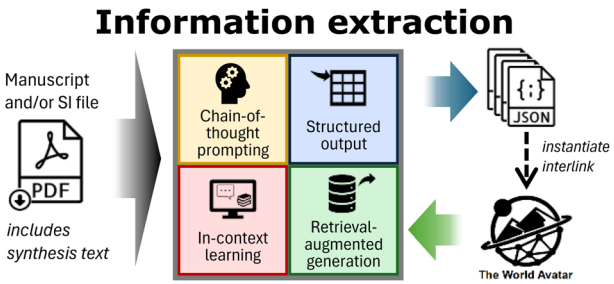

Extraction of chemical synthesis information using the World Avatar

Simon D. Rihm, Fabio Saluz, Aleksandar Kondinski, Jiaru Bai, Patrick W. V. Butler, Sebastian Mosbach, Jethro Akroyd and Markus Kraft*

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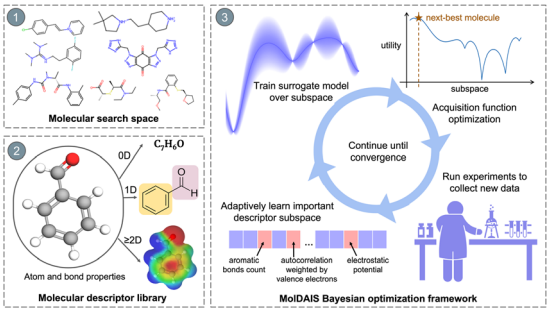
Adaptive subspace Bayesian optimization over molecular descriptor libraries for data-efficient chemical design

Farshud Sorourifar, Thomas Banker and Joel A. Paulson*



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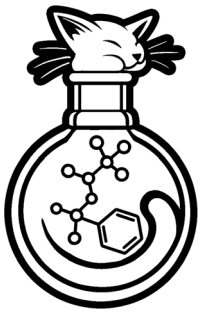
Moment of inertia as a simple shape descriptor for diffusion-based shape-constrained molecular generation

Denis Sapegin,* Fedor Bakharev, Dmitriy Krupenya, Azamat Gafurov, Konstantin Pildish and Joseph C. Bear*



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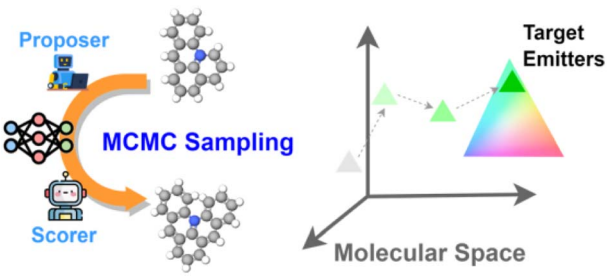
Generative AI-powered inverse design for tailored narrowband molecular emitters

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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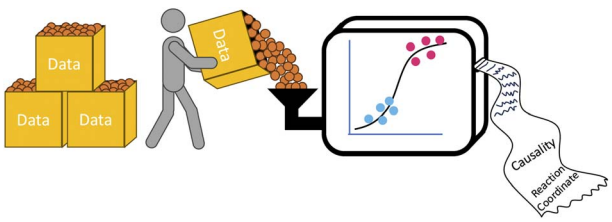
Coupling causality and interpretable machine learning to reveal the reaction coordinate of C–N coupling with a supramolecular Cu-calix[8]arene catalyst

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



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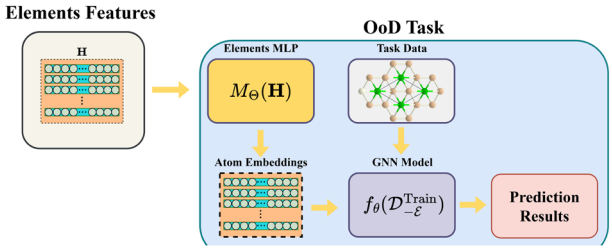

Beyond training data: how elemental features enhance ML-based formation energy predictions

Hamed Mahdavi,* Vasant Honavar and Dane Morgan

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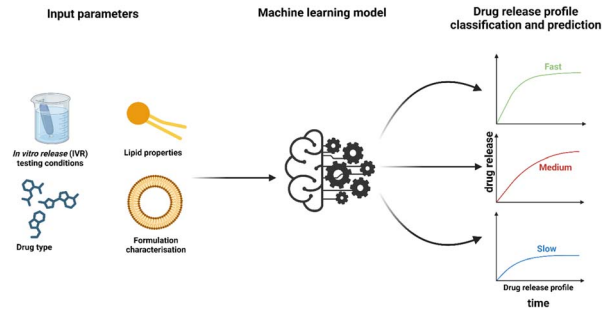

A machine learning workflow to accelerate the design of *in vitro* release tests from liposomes

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

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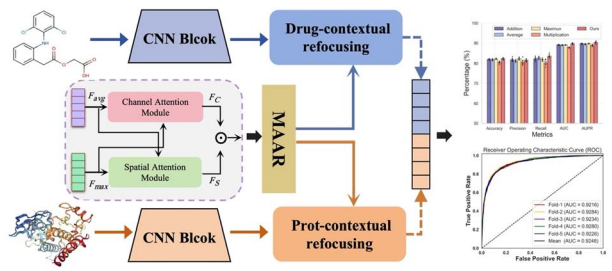

MAARDTI: a multi-perspective attention aggregation model for the prediction of drug–target interactions

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

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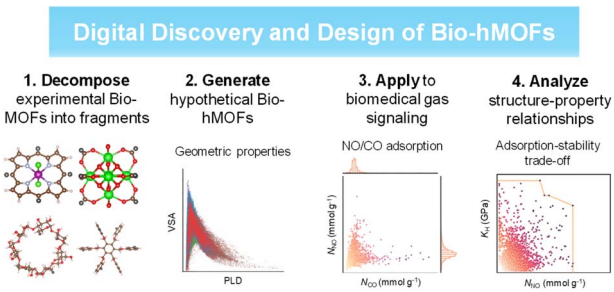

Digital design and discovery of biological metal–organic frameworks for gas signaling

Yifei Yue, Athulya S. Palakkal, Saad Aldin Mohamed and Jianwen Jiang*

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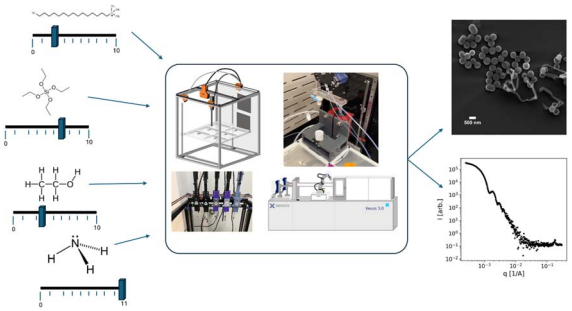
Accelerated sol–gel synthesis of nanoporous silica *via* integrated small angle X-ray scattering with an open-source automation platform

Brenden Pelkie, Chi Yuet Yung, Zachery R. Wylie and Lilo D. Pozzo*



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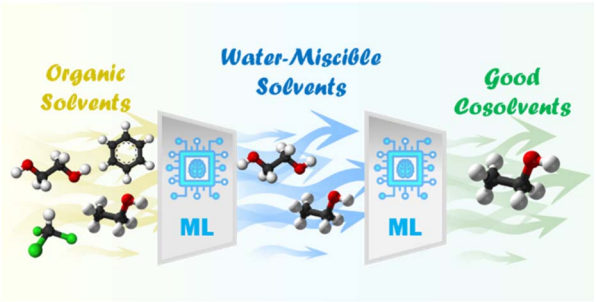
Predicting aqueous and organic solubilities with machine learning: a workflow for identifying organic cosolvents

Maurycy Krzyżanowski, Sirazam Munira Aishee, Nirala Singh* and Bryan R. Goldsmith*



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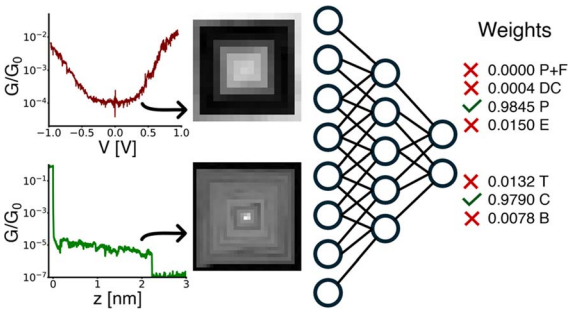
"Twisting" the data: a universal machine-learning approach to classify single-molecule curves and beyond

C. Roldán-Piñero,* M. Teresa González, Pablo M. Olmos, Linda A. Zotti and Edmund Leary*



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