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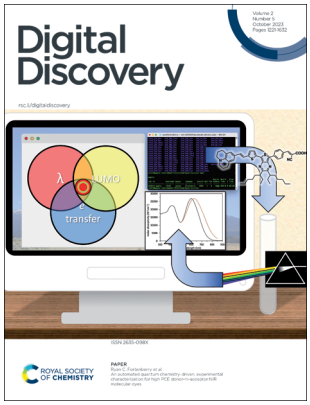

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See Ryan C. Fortenberry *et al.*, pp. 1269–1288.
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Inside cover
See Jean-Louis Reymond *et al.*, pp. 1289–1296. Image reproduced by permission of Markus Orsi from *Digital Discovery*, 2023, **2**, 1289.
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14 examples of how LLMs can transform materials science and chemistry: a reflection on a large language model hackathon

K. M. Jablonka,* Q. Ai, A. Al-Feghali, S. Badhwar, J. D. Bocarsly, A. M. Bran, S. Bringuier, L. C. Brinson, K. Choudhary, D. Circi, S. Cox, W. A. de Jong, M. L. Evans, N. Gastellu, J. Genzling, M. V. Gil, A. K. Gupta, Z. Hong, A. Imran, S. Kruschwitz, A. Labarre, J. Lála, T. Liu, S. Ma, S. Majumdar, G. W. Merz, N. Moitessier, E. Moubarak, B. Mouriño, B. Pelkie, M. Pieler, M. Ramos, B. Ranković, S. G. Rodriques, J. N. Sanders, P. Schwaller, M. Schwarting, J. Shi, B. Smit, B. E. Smith, J. Van Herck, C. Völker, L. Ward, S. Warren, B. Weiser, S. Zhang, X. Zhang, G. A. Zia, A. Scourtas, K. J. Schmidt, I. Foster, A. D. White and B. Blaiszik*

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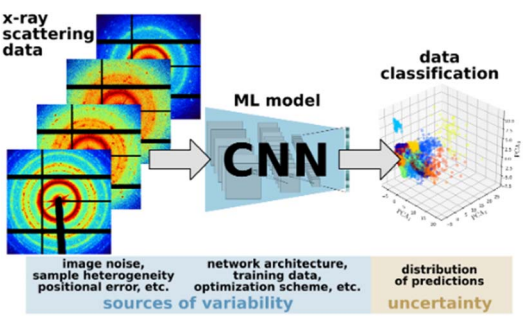
A rigorous uncertainty-aware quantification framework is essential for reproducible and replicable machine learning workflows

Line Pouchard, Kristofer G. Reyes, Francis J. Alexander and Byung-Jun Yoon*



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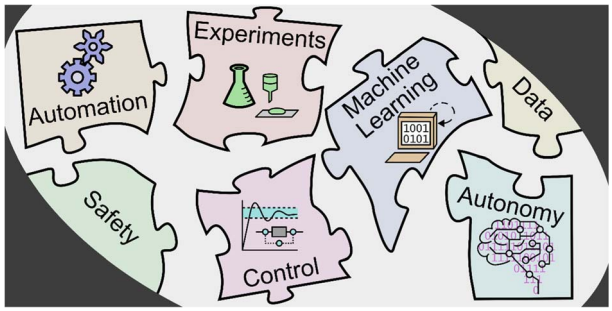
Integrating autonomy into automated research platforms

Richard B. Canty, Brent A. Koscher, Matthew A. McDonald and Klavs F. Jensen*



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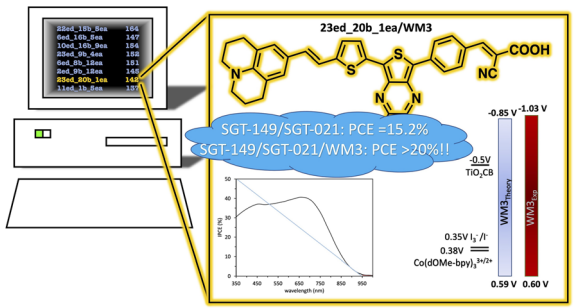
An automated quantum chemistry-driven, experimental characterization for high PCE donor–π–acceptor NIR molecular dyes

Taylor J. Santaloci, William E. Meador, Austin M. Wallace, E. Michael Valencia, Blake N. Rogers, Jared H. Delcamp and Ryan C. Fortenberry*



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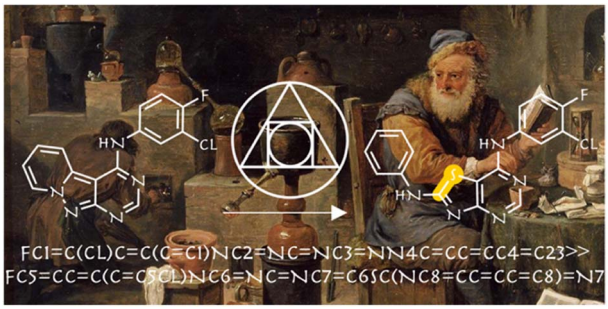
Alchemical analysis of FDA approved drugs

Markus Orsi, Daniel Probst, Philippe Schwaller and Jean-Louis Reymond*



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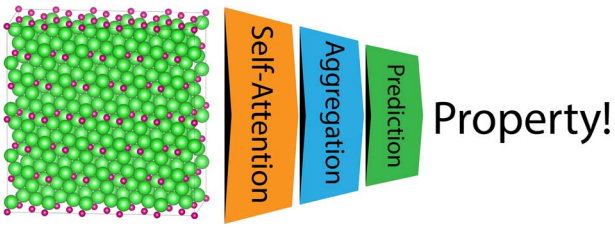
Site-Net: using global self-attention and real-space supercells to capture long-range interactions in crystal structures

Michael Moran, Michael W. Gaultois,* Vladimir V. Gusev and Matthew J. Rosseinsky



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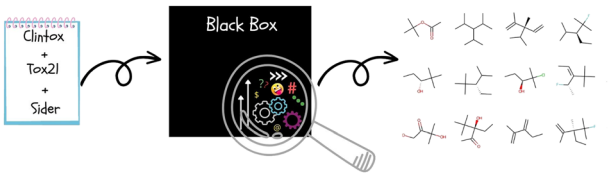

Generating structural alerts from toxicology datasets using the local interpretable model-agnostic explanations method

Cayque Monteiro Castro Nascimento, Paloma Guimarães Moura and Andre Silva Pimentel*

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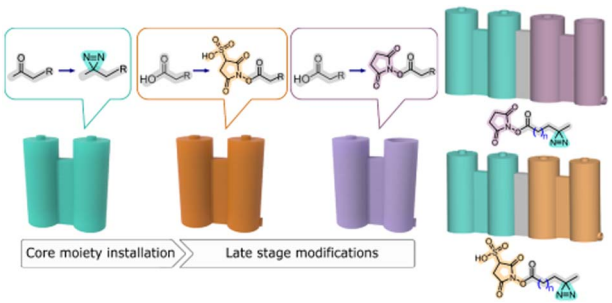

Digital design and 3D printing of reactionware for on demand synthesis of high value probes

Przemyslaw Frei, Philip J. Kitson, Alexander X. Jones and Leroy Cronin*

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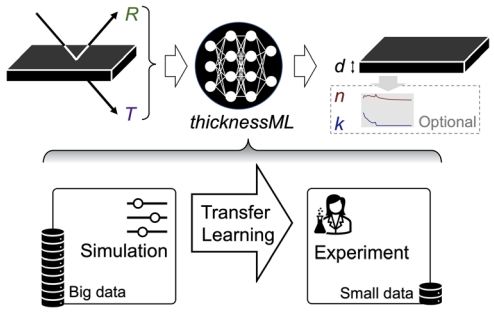

Tackling data scarcity with transfer learning: a case study of thickness characterization from optical spectra of perovskite thin films

Siyu Isaac Parker Tian, Zekun Ren, Selvaraj Venkataraj, Yuanhang Cheng, Daniil Bash, Felipe Oviedo, J. Senthilnath, Vijila Chellappan, Yee-Fun Lim, Armin G. Aberle, Benjamin P. MacLeod, Fraser G. L. Parlane, Curtis P. Berlinguette, Qianxiao Li, Tonio Buonassisi* and Zhe Liu

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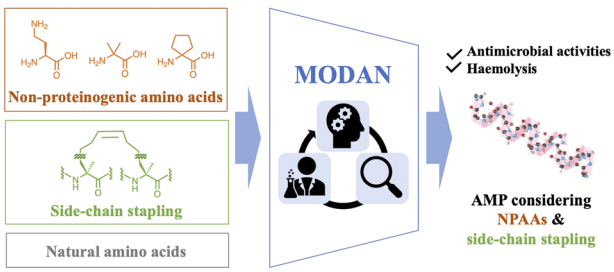

Design of antimicrobial peptides containing non-proteinogenic amino acids using multi-objective Bayesian optimisation

Yuki Murakami, Shoichi Ishida, Yosuke Demizu and Kei Terayama*

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Deep representation learning determines drug mechanism of action from cell painting images

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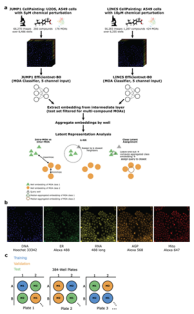

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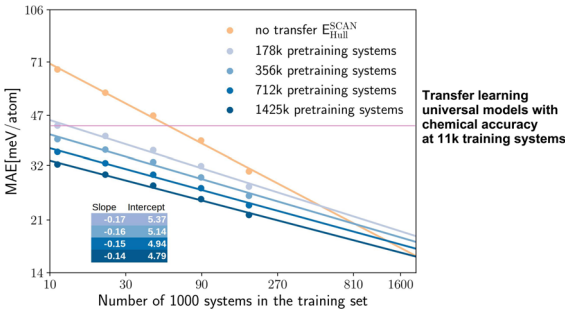
Transfer learning on large datasets for the accurate prediction of material properties

Noah Hoffmann, Jonathan Schmidt, Silvana Botti and Miguel A. L. Marques*



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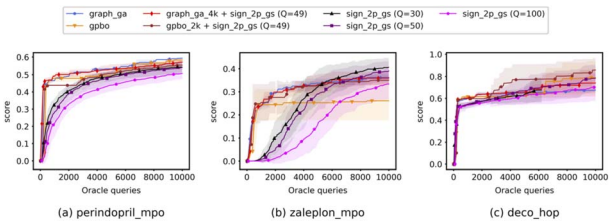
Understanding and improving zeroth-order optimization methods on AI-driven molecule optimization

Elvin Lo and Pin-Yu Chen*



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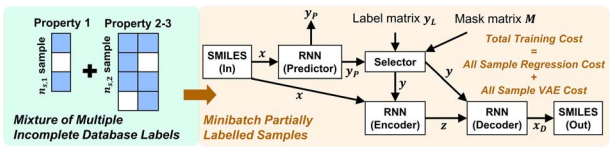
Multi-constraint molecular generation using sparsely labelled training data for localized high-concentration electrolyte diluent screening

Jonathan P. Mailoa,* Xin Li, Jiezhong Qiu and Shengyu Zhang*



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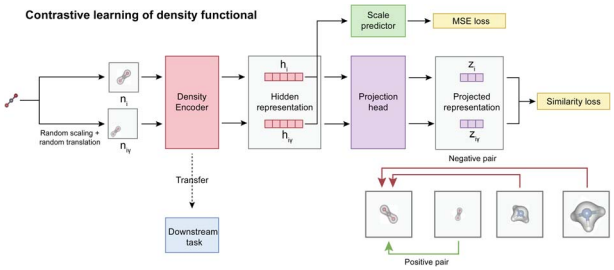

Incorporation of density scaling constraint in density functional design *via* contrastive representation learning

Weiyi Gong, Tao Sun, Hexin Bai, Shah Tanvir ur Rahman Chowdhury, Peng Chu, Anoj Aryal, Jie Yu, Haibin Ling,* John P. Perdew* and Qimin Yan*

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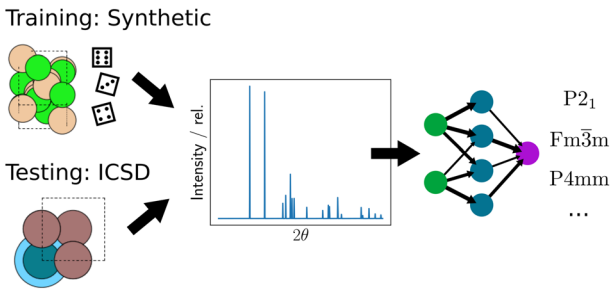

Neural networks trained on synthetically generated crystals can extract structural information from ICSD powder X-ray diffractograms

Henrik Schopmans, Patrick Reiser and Pascal Friederich*

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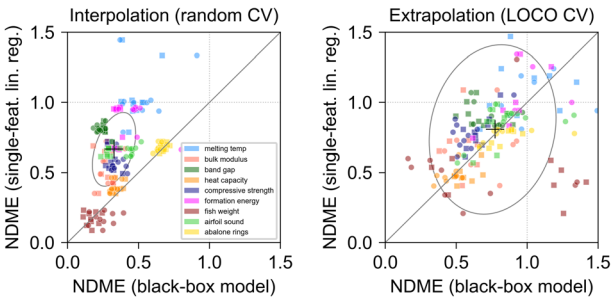

Interpretable models for extrapolation in scientific machine learning

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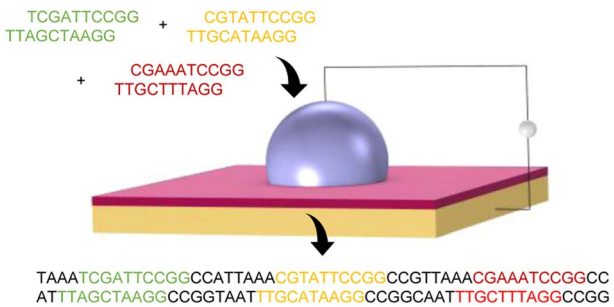

Automated routing of droplets for DNA storage on a digital microfluidics platform

Ajay Manicka, Andrew Stephan, Sriram Chari, Gemma Mendonsa, Peyton Okubo, John Stolzberg-Schray, Anil Reddy and Marc Riedel

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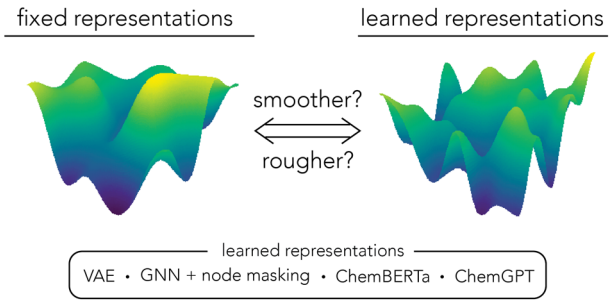
Evaluating the roughness of structure–property relationships using pretrained molecular representations

David E. Graff, Edward O. Pyzer-Knapp, Kirk E. Jordan, Eugene I. Shakhnovich and Connor W. Coley



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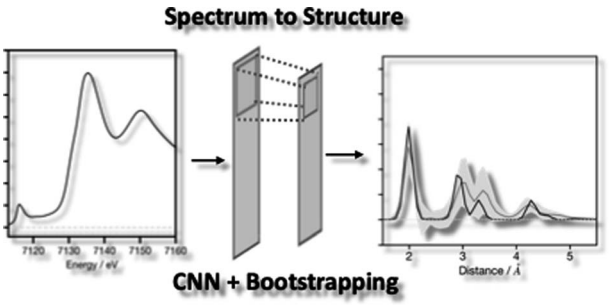
Towards the automated extraction of structural information from X-ray absorption spectra

Tudur David,* Nik Khadijah Nik Aznan, Kathryn Garside and Thomas Penfold



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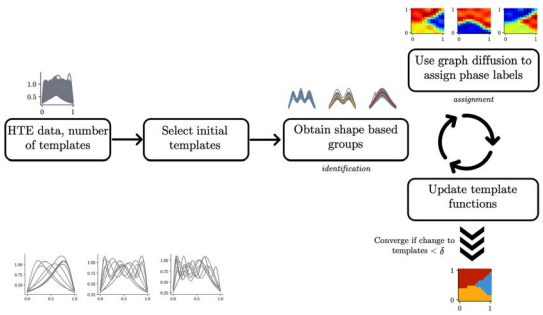
Metric geometry tools for automatic structure phase map generation

Kiran Vaddi,* Karen Li and Lilo D. Pozzo



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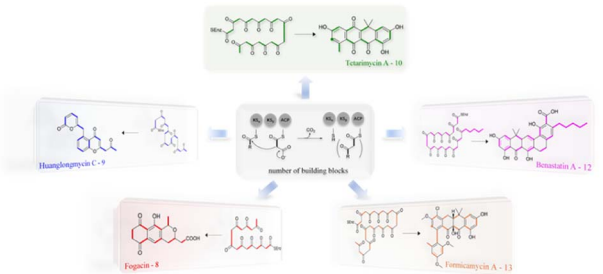
A deep learning model for type II polyketide natural product prediction without sequence alignment

Jiaquan Huang, Qiandi Gao, Ying Tang, Yaxin Wu, Heqian Zhang* and Zhiwei Qin*



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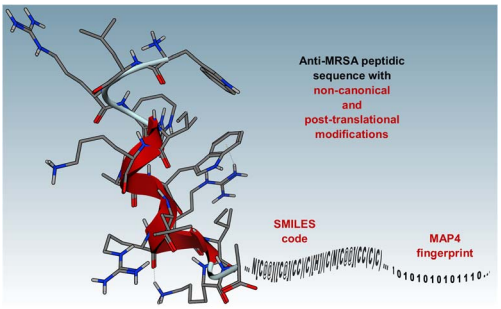

Mapping the structure–activity landscape of non-canonical peptides with MAP4 fingerprinting

Edgar López-López,* Oscar Robles, Fabien Plisson and José L. Medina-Franco*

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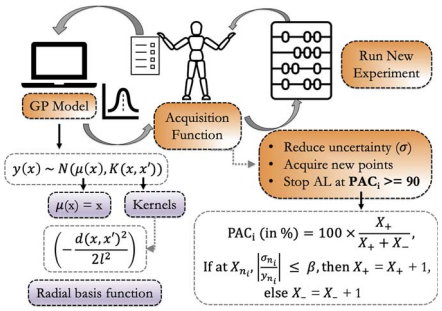

Active learning for efficient navigation of multi-component gas adsorption landscapes in a MOF

Krishnendu Mukherjee, Etinosa Osaro and Yamil J. Colón*

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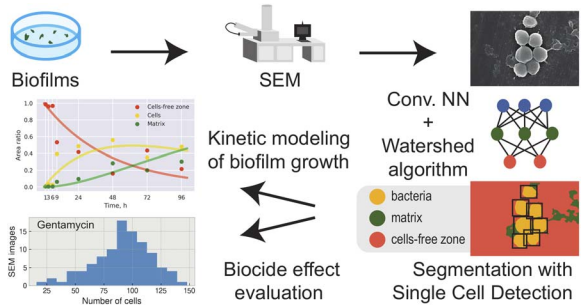

Digital biology approach for macroscale studies of biofilm growth and biocide effects with electron microscopy

Konstantin S. Kozlov, Daniil A. Boiko, Elena V. Detusheva, Konstantin V. Detushev, Evgeniy O. Pentsak, Anatoly N. Vereshchagin and Valentine P. Ananikov*

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Go with the flow: deep learning methods for autonomous viscosity estimations

Michael Walker, Gabriella Pizzuto, Hatem Fakhruldeen and Andrew I. Cooper*

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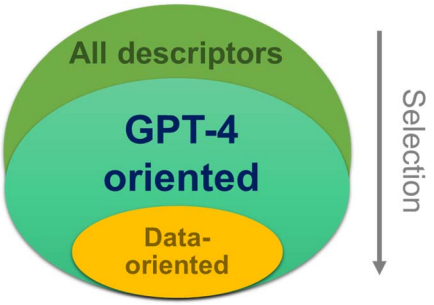
Using GPT-4 in parameter selection of polymer informatics: improving predictive accuracy amidst data scarcity and 'Ugly Duckling' dilemma

Kan Hatakeyama-Sato,* Seigo Watanabe, Naoki Yamane, Yasuhiko Igarashi and Kenichi Oyaizu*



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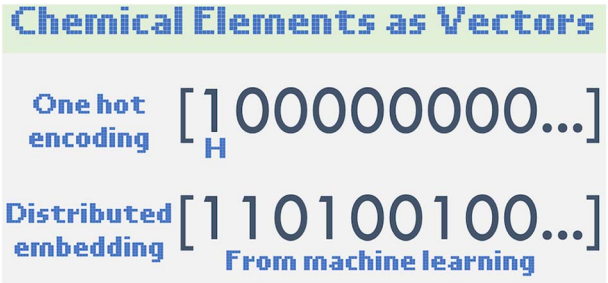
Element similarity in high-dimensional materials representations

Anthony Onwuli, Ashish V. Hegde, Kevin V. T. Nguyen, Keith T. Butler* and Aron Walsh*



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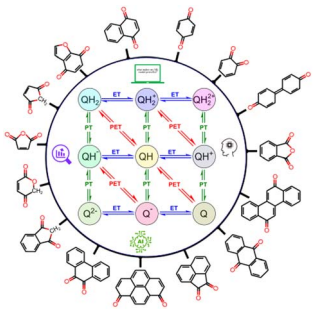
Density functional theory and machine learning for electrochemical square-scheme prediction: an application to quinone-type molecules relevant to redox flow batteries

Arsalan Hashemi,* Reza Khakpour, Amir Mahdian, Michael Busch, Pekka Peljo and Kari Laasonen



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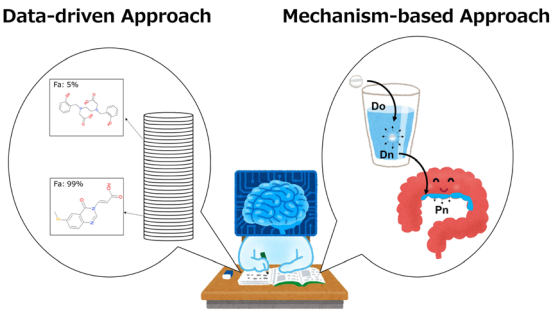
Combined data-driven and mechanism-based approaches for human-intestinal-absorption prediction in the early drug-discovery stage

Koichi Handa,* Sakae Sugiyama, Michiharu Kageyama and Takeshi Iijima



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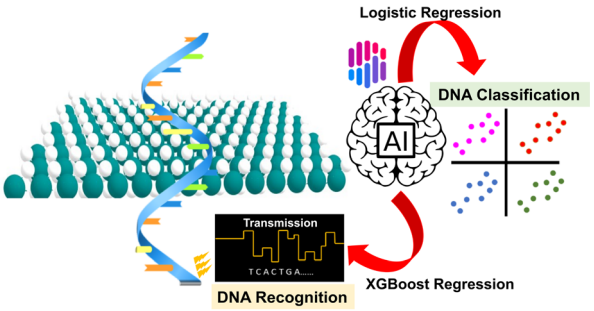
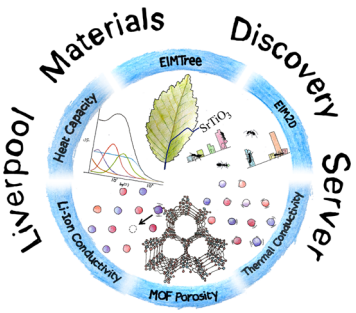


Artificial intelligence aided recognition and classification of DNA nucleotides using MoS_2 nanochannels

Sneha Mittal, Souvik Manna, Milan Kumar Jena and Biswarup Pathak*

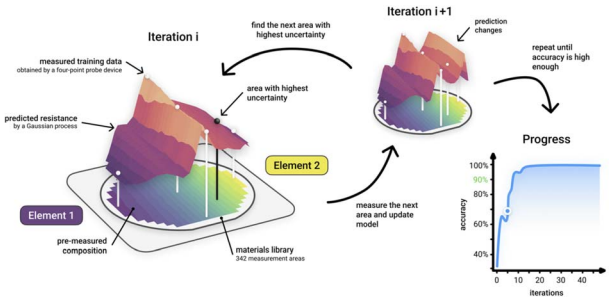
1601



The Liverpool materials discovery server: a suite of computational tools for the collaborative discovery of materials

Samantha Durdy, Cameron J. Hargreaves, Mark Dennison, Benjamin Wagg, Michael Moran, Jon A. Newnham, Michael W. Gaultois, Matthew J. Rosseinsky and Matthew S. Dyer*

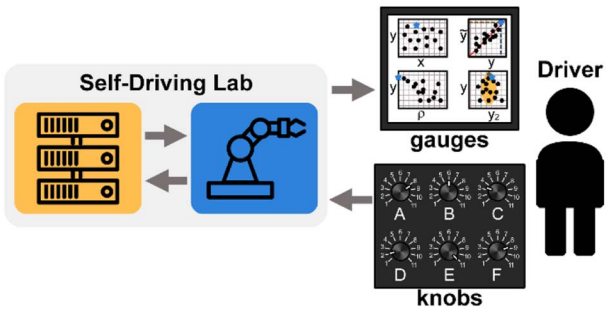
1612



Speeding up high-throughput characterization of materials libraries by active learning: autonomous electrical resistance measurements

Felix Thelen, Lars Banko, Rico Zehl, Sabrina Baha and Alfred Ludwig*

1620



Driving school for self-driving labs

Kelsey L. Snapp and Keith A. Brown*

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