

# Digital Discovery

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## IN THIS ISSUE

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**Cover**  
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.  
Background: David Teniers the Younger, "The Alchemist". Mauritshuis, The Hague.

## PERSPECTIVES

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### 14 examples of how LLMs can transform materials science and chemistry: a reflection on a large language model hackathon

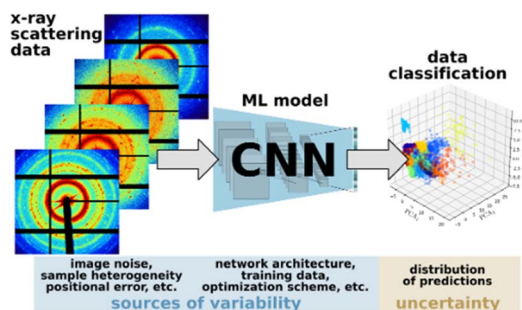
K. M. Jablonka,\* Q. Ai, A. Al-Feghali, S. Badhwar, J. D. Bocarsly, A. M. Bran, S. Bringuier, L. C. Brinson, K. Choudhary, D. Circi, S. Cox, W. A. de Jong, M. L. Evans, N. Gastellu, J. Genzling, M. V. Gil, A. K. Gupta, Z. Hong, A. Imran, S. Kruschwitz, A. Labarre, J. Lála, T. Liu, S. Ma, S. Majumdar, G. W. Merz, N. Moitessier, E. Moubarak, B. Mouriño, B. Pelkie, M. Pieler, M. Ramos, B. Ranković, S. G. Rodrigues, 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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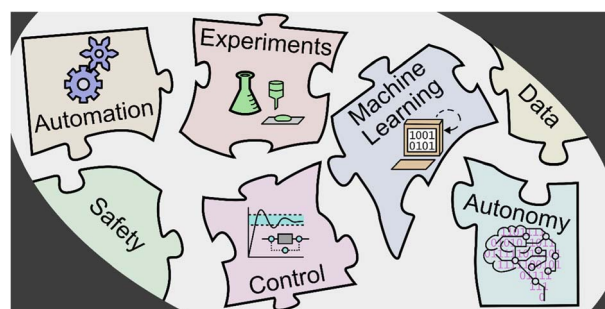


## PERSPECTIVES

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## Integrating autonomy into automated research platforms

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

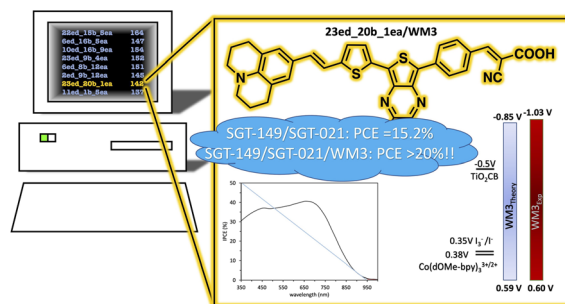


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An automated quantum chemistry-driven, experimental characterization for high PCE donor- $\pi$ -acceptor NIR molecular dyes

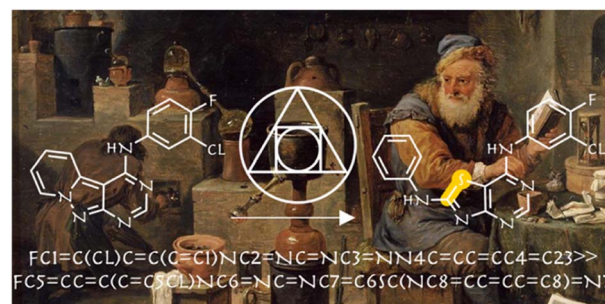
Taylor J. Santaloci, William E. Meador, Austin M. Wallace, E. Michael Valencia, Blake N. Rogers, Jared H. Delcamp and Ryan C. Fortenberry\*



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## Alchemical analysis of FDA approved drugs

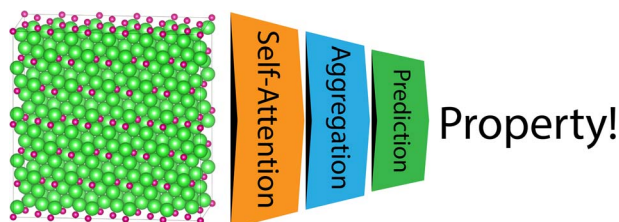
Markus Orsi, Daniel Probst, Philippe Schwaller and Jean-Louis Reymond\*



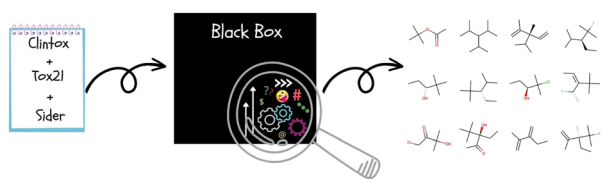
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## Site-Net: using global self-attention and real-space supercells to capture long-range interactions in crystal structures

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



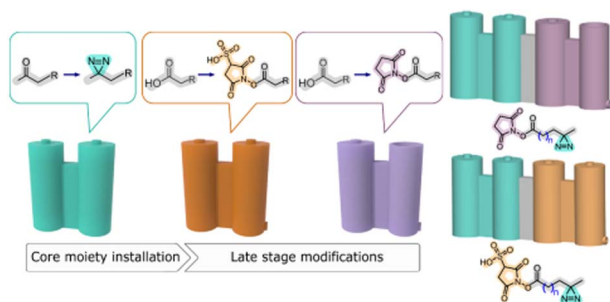
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### Generating structural alerts from toxicology datasets using the local interpretable model-agnostic explanations method

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

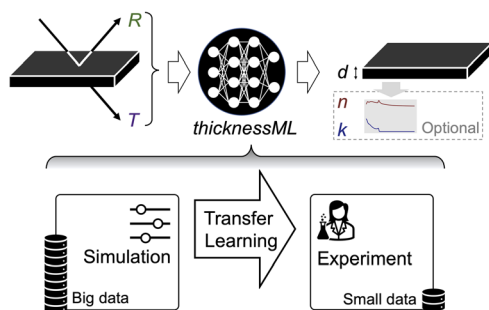
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### Digital design and 3D printing of reactionware for on demand synthesis of high value probes

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

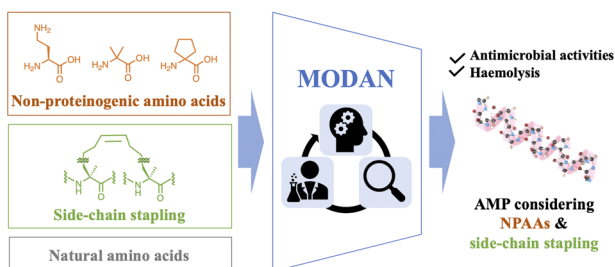
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### Tackling data scarcity with transfer learning: a case study of thickness characterization from optical spectra of perovskite thin films

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

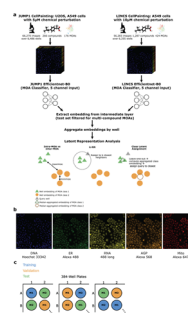
Yuki Murakami, Shoichi Ishida, Yosuke Demizu and Kei Terayama\*



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

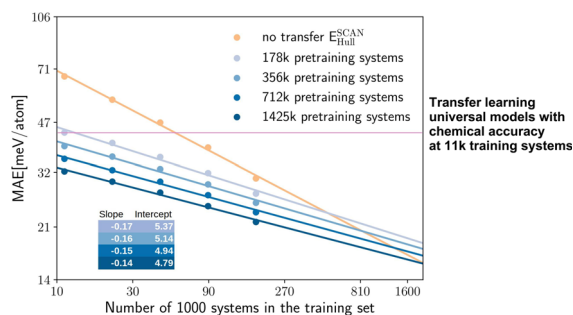
Daniel R. Wong,<sup>\*</sup> David J. Logan, Santosh Hariharan, Robert Stanton, Djork-Arné Clevert and Andrew Kiruluta



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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<sup>\*</sup>

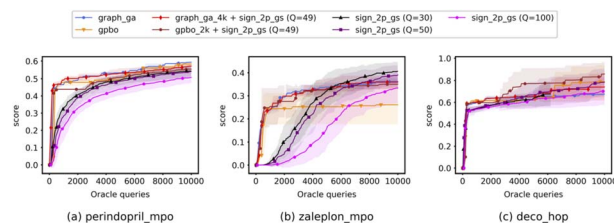


Transfer learning universal models with chemical accuracy at 11k training systems

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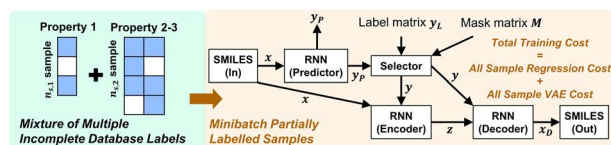
Elvin Lo and Pin-Yu Chen<sup>\*</sup>



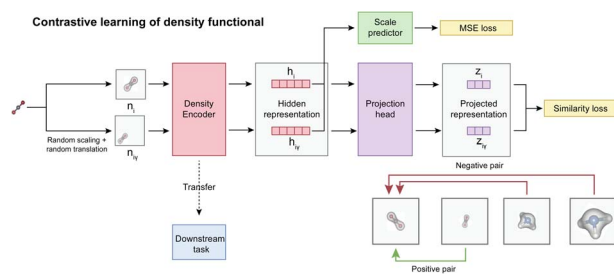
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## Multi-constraint molecular generation using sparsely labelled training data for localized high-concentration electrolyte diluent screening

Jonathan P. Mailoa,<sup>\*</sup> Xin Li, Jiezhong Qiu and Shengyu Zhang<sup>\*</sup>



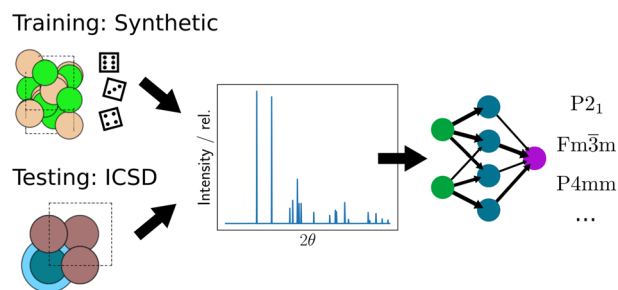
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### Incorporation of density scaling constraint in density functional design via contrastive representation learning

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\*

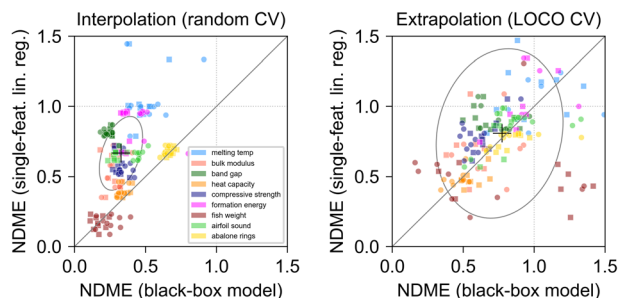
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### Neural networks trained on synthetically generated crystals can extract structural information from ICSD powder X-ray diffractograms

Henrik Schopmans, Patrick Reiser and Pascal Friederich\*

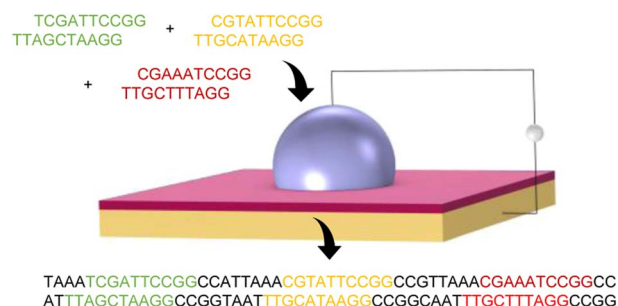
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Eric S. Muckley, James E. Saal,\* Bryce Meredig, Christopher S. Roper and John H. Martin

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

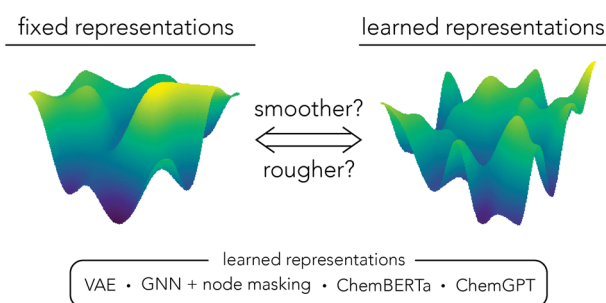
Ajay Manicka, Andrew Stephan, Sriram Chari, Gemma Mendonsa, Peyton Okubo, John Stolzberg-Schray, Anil Reddy and Marc Riedel



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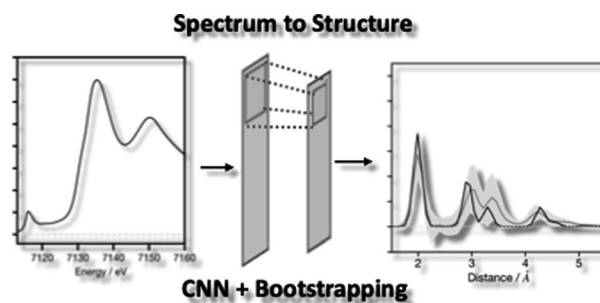
David E. Graff, Edward O. Pyzer-Knapp, Kirk E. Jordan, Eugene I. Shakhnovich and Connor W. Coley



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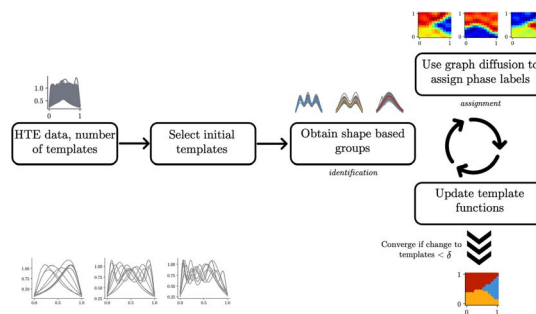
Tudur David,\* Nik Khadijah Nik Aznan, Kathryn Garside and Thomas Penfold



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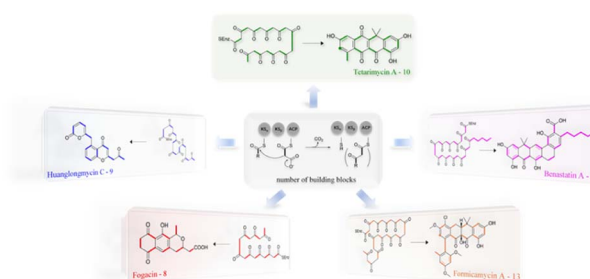
Kiran Vaddi,\* Karen Li and Lilo D. Pozzo



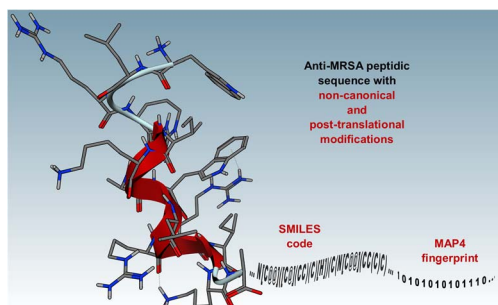
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## A deep learning model for type II polyketide natural product prediction without sequence alignment

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



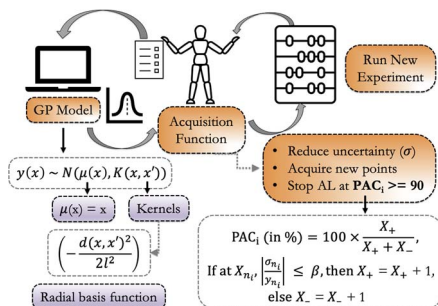
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Edgar López-López,<sup>\*</sup> Oscar Robles, Fabien Plisson and José L. Medina-Franco<sup>\*</sup>

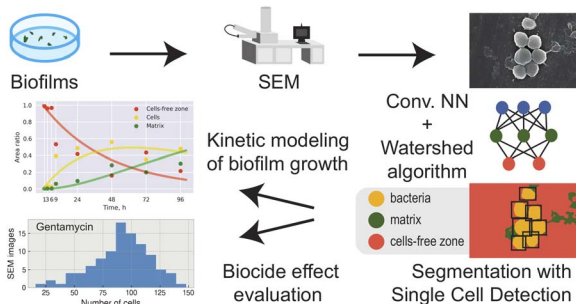
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### Active learning for efficient navigation of multi-component gas adsorption landscapes in a MOF

Krishnendu Mukherjee, Etinosa Osaro and Yamil J. Colón<sup>\*</sup>

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### Digital biology approach for macro-scale 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<sup>\*</sup>

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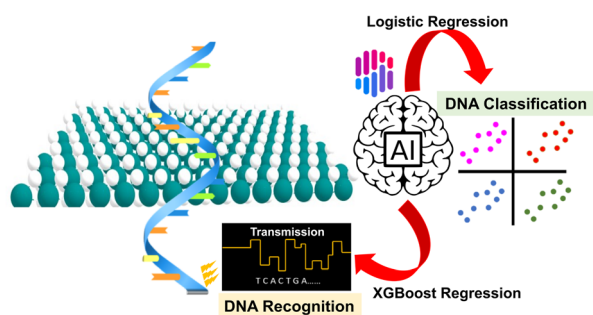
### Go with the flow: deep learning methods for autonomous viscosity estimations

Michael Walker, Gabriella Pizzuto, Hatem Fakhrudeen and Andrew I. Cooper<sup>\*</sup>





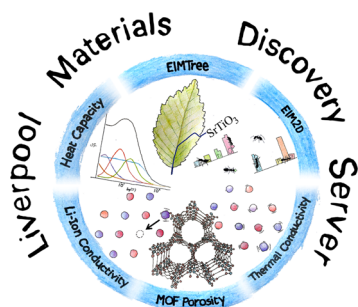
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## Artificial intelligence aided recognition and classification of DNA nucleotides using MoS<sub>2</sub> nanochannels

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

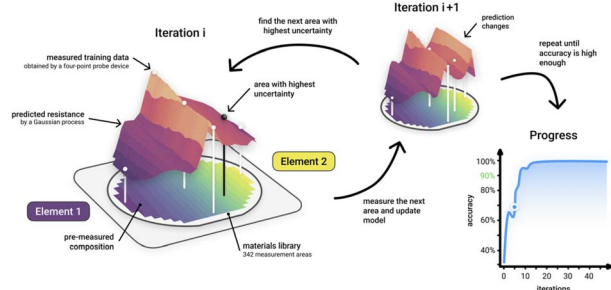
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## The Liverpool materials discovery server: a suite of computational tools for the collaborative discovery of materials

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

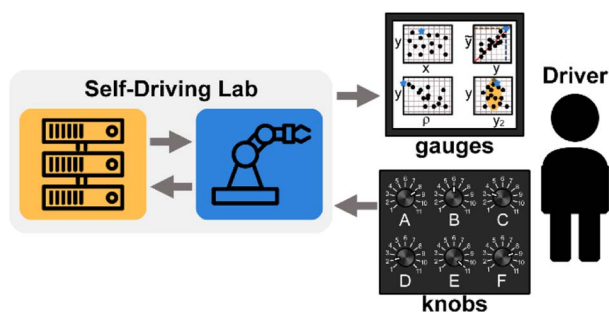
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## Speeding up high-throughput characterization of materials libraries by active learning: autonomous electrical resistance measurements

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

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## Driving school for self-driving labs

Kelsey L. Snapp and Keith A. Brown\*

