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# Digital Discovery

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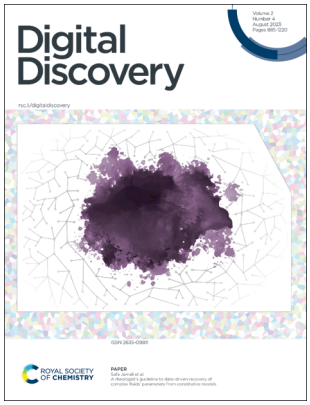
## IN THIS ISSUE

ISSN 2635-098X CODEN DDIIAI 2(4) 885–1220 (2023)

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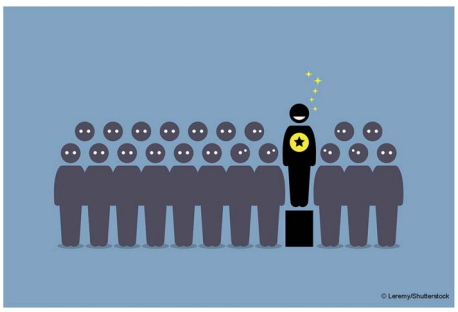

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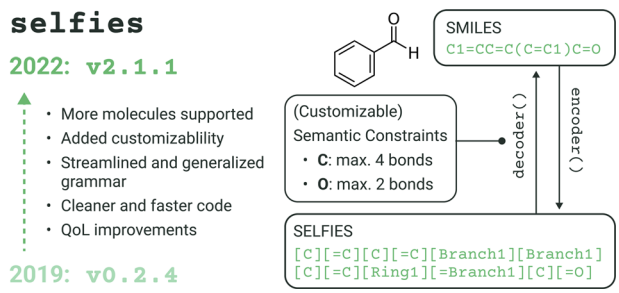
**Recent advances in the self-referencing embedded strings (SELFIES) library**

Alston Lo,* Robert Pollice, AkshatKumar Nigam, Andrew D. White, Mario Krenn and Alán Aspuru-Guzik



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## COMMUNICATION

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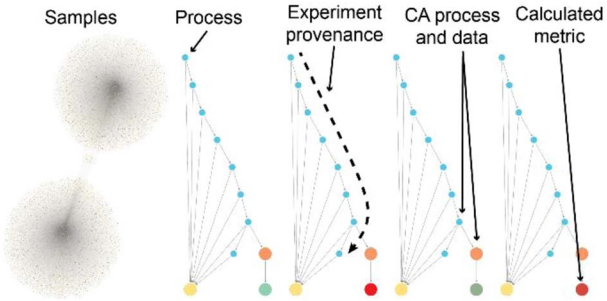
**The materials experiment knowledge graph**

Michael J. Statt,* Brian A. Rohr,* Dan Guevarra, Ja'Nya Breeden, Santosh K. Suram and John M. Gregoire*

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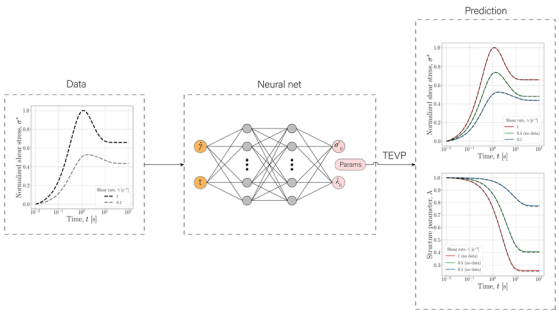
**A rheologist's guideline to data-driven recovery of complex fluids' parameters from constitutive models**

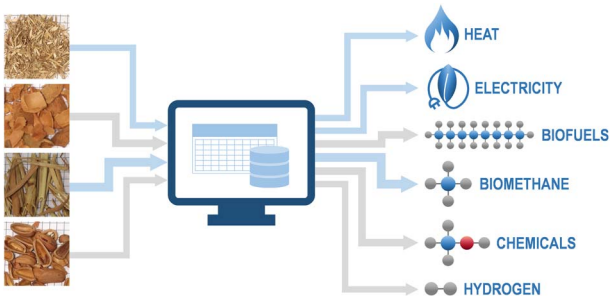
Milad Saadat, Deepak Mangal and Safa Jamali*




929

**Biomass to energy: a machine learning model for optimum gasification pathways**

María Victoria Gil,* Kevin Maik Jablonka, Susana Garcia, Covadonga Pevida and Berend Smit*

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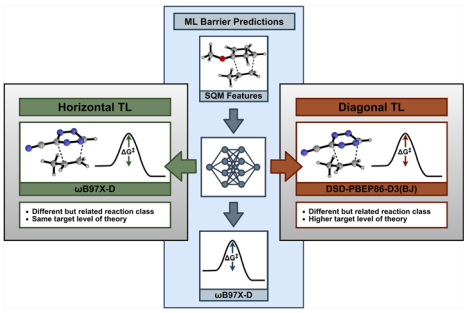
**Machine learning reaction barriers in low data regimes: a horizontal and diagonal transfer learning approach**

Samuel G. Espley, Elliot H. E. Farrar, David Buttar, Simone Tomasi and Matthew N. Grayson*

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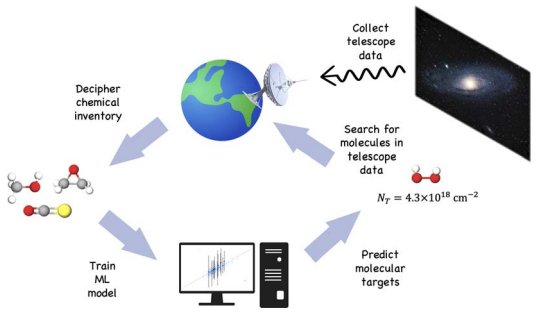


## Implementation of rare isotopologues into machine learning of the chemical inventory of the solar-type protostellar source IRAS 16293-2422

Zachary T. P. Fried,* Kin Long Kelvin Lee, Alex N. Byrne and Brett A. McGuire*

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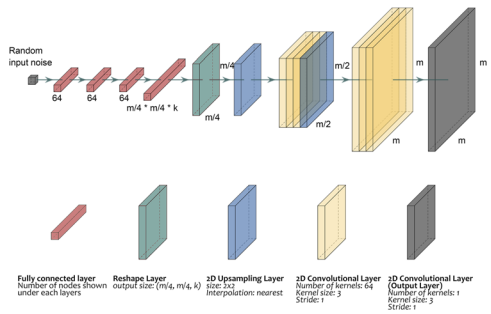


## A scalable neural network architecture for self-supervised tomographic image reconstruction

Hongyang Dong, Simon D. M. Jacques, Winfried Kockelmann, Stephen W. T. Price, Robert Emberson, Dorota Matras, Yaroslav Odarchenko, Vesna Middelkoop, Athanasios Giokaris, Olof Gutowski, Ann-Christin Dippel, Martin von Zimmermann, Andrew M. Beale, Keith T. Butler* and Antonis Vamvakeros*

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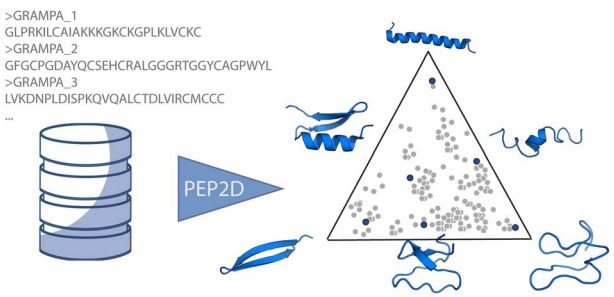


## Benchmarking protein structure predictors to assist machine learning-guided peptide discovery

Victor Daniel Aldas-Bulos and Fabien Plisson*

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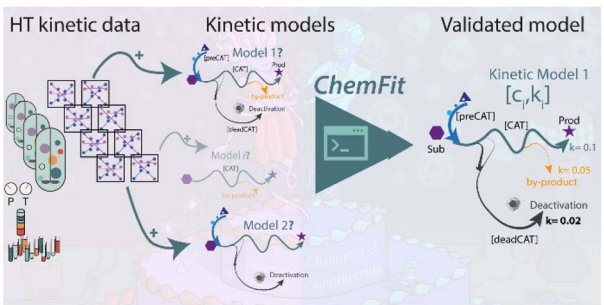


## Model-based evaluation and data requirements for parallel kinetic experimentation and data-driven reaction identification and optimization

Nathan Jiscoot, Evgeny A. Uslamin* and Evgeny A. Pidko*

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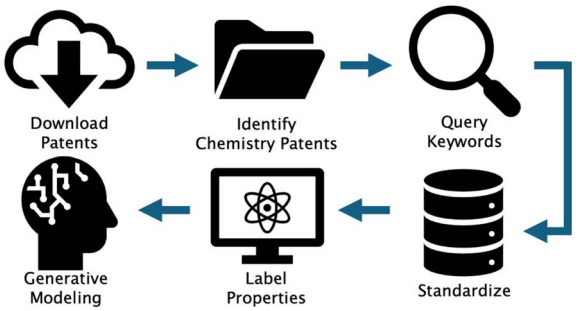
**Automated patent extraction powers generative modeling in focused chemical spaces**

Akshay Subramanian, Kevin P. Greenman, Alexis Gervaix, Tzuhsiung Yang and Rafael Gómez-Bombarelli*

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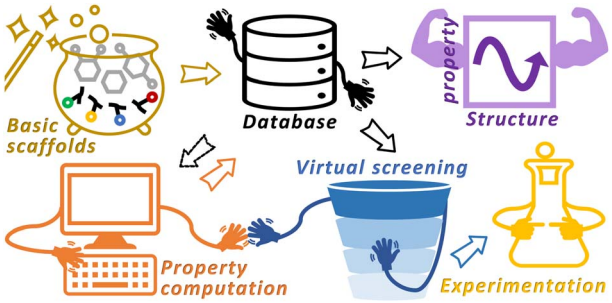
**Discovery of lead quinone cathode materials for Li-ion batteries**

Xuan Zhou, Abhishek Khetan, Jie Zheng, Mark Huijben, René A. J. Janssen and Süleyman Er*

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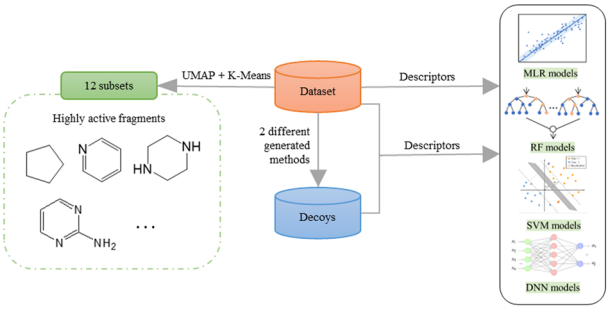
**A SAR and QSAR study on cyclin dependent kinase 4 inhibitors using machine learning methods**

Xiaoyang Pang, Yunyang Zhao, Guo Li, Jianrong Liu* and Aixia Yan*

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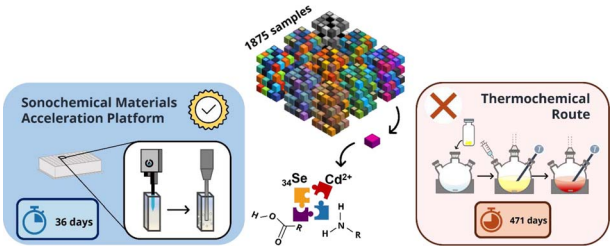
**A high-throughput workflow for the synthesis of CdSe nanocrystals using a sonochemical materials acceleration platform**

Maria Politi, Fabio Baum, Kiran Vaddi, Edwin Antonio, Joshua Vasquez, Brittany P. Bishop, Nadya Peek, Vincent C. Holmberg and Lilo D. Pozzo*

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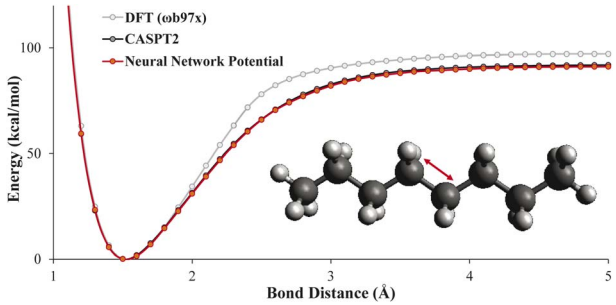


**Neural network potentials for reactive chemistry: CASPT2 quality potential energy surfaces for bond breaking**

Quin H. Hu, Andrew M. Johannesen, Daniel S. Graham and Jason D. Goodpaster*

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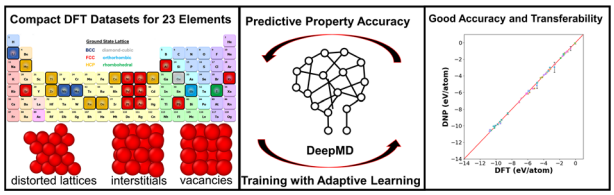


**Highly transferable atomistic machine-learning potentials from curated and compact datasets across the periodic table**

Christopher M. Andolina and Wissam A. Saidi*

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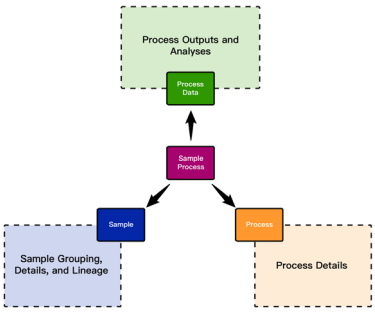


**ESAMP: event-sourced architecture for materials provenance management and application to accelerated materials discovery**

Michael J. Statt,* Brian A. Rohr, Kris Brown, Dan Guevarra, Jens Hummelshøj, Linda Hung, Abraham Anapolsky, John M. Gregoire* and Santosh K. Suram*

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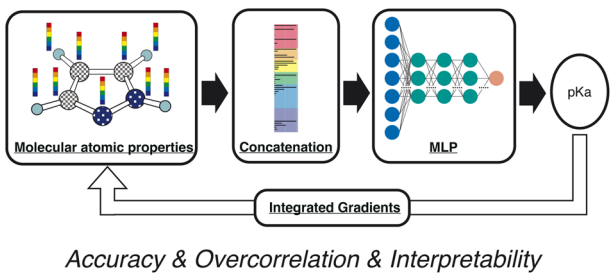


**Feature selection in molecular graph neural networks based on quantum chemical approaches**

Daisuke Yokogawa* and Kayo Suda

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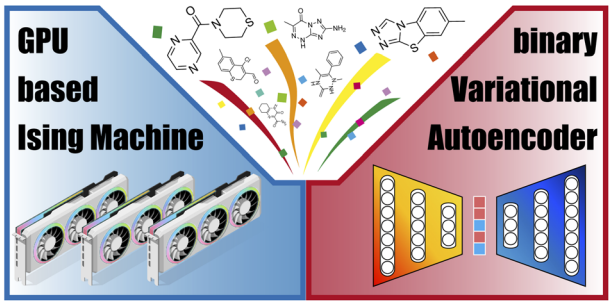
**Chemical design with GPU-based Ising machines**

Zetian Mao, Yoshiki Matsuda, Ryo Tamura* and Koji Tsuda*

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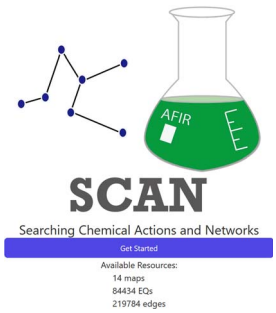
**Searching chemical action and network (SCAN): an interactive chemical reaction path network platform**

Mikael Kuwahara, Yu Harabuchi, Satoshi Maeda,* Jun Fujima* and Keisuke Takahashi*

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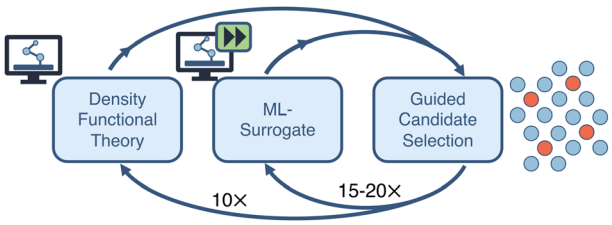
**By how much can closed-loop frameworks accelerate computational materials discovery?**

Lance Kavalsky, Vinay I. Hegde, Eric Muckley, Matthew S. Johnson, Bryce Meredig* and Venkatasubramanian Viswanathan*

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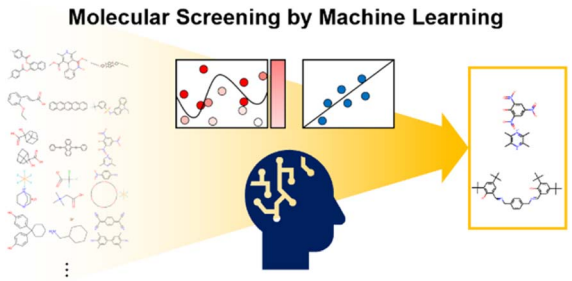
**Molecular screening for solid–solid phase transitions by machine learning**

Daisuke Takagi, Kazuki Ishizaki, Toru Asahi and Takuya Taniguchi*

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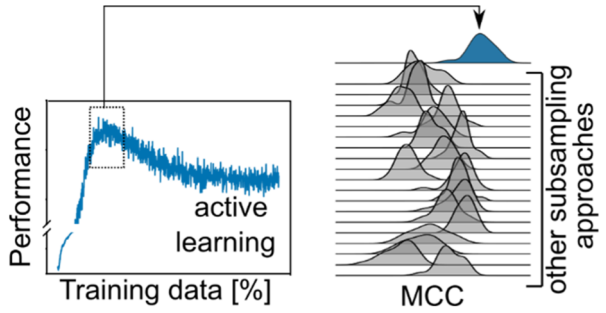


**Improving molecular machine learning through adaptive subsampling with active learning**

Yujing Wen, Zhixiong Li, Yan Xiang and Daniel Reker*

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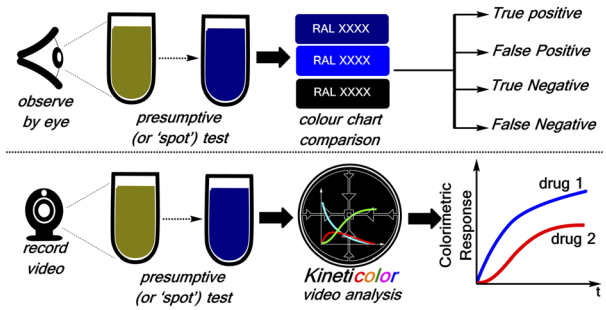


**Teaching old presumptive tests new digital tricks with computer vision for forensic applications**

Nathalie Bugeja, Cameron Oliver, Nicole McGrath, Jake McGuire, Chunhui Yan, Felicity Carlysle-Davies and Marc Reid*

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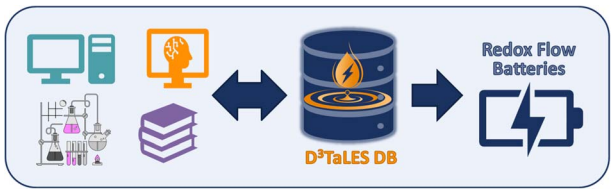


**Towards a comprehensive data infrastructure for redox-active organic molecules targeting non-aqueous redox flow batteries**

Rebekah Duke, Vinayak Bhat, Parker Sornberger, Susan A. Odom and Chad Risko*

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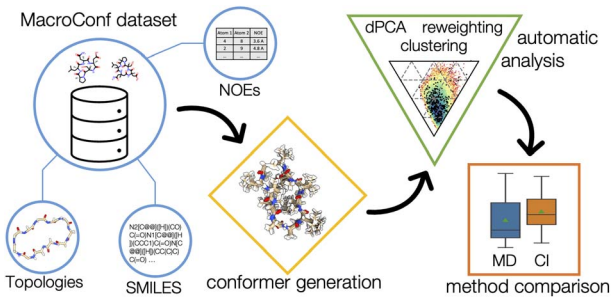


**MacroConf – dataset & workflows to assess cyclic peptide solution structures**

Daniel Crusius, Jason R. Schnell, Flaviu Cipcigan and Philip C. Biggin*

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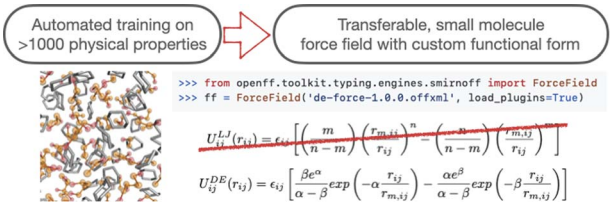
## A transferable double exponential potential for condensed phase simulations of small molecules

Joshua T. Horton, Simon Boothroyd, Pavan Kumar Behara, David L. Mobley and Daniel J. Cole*

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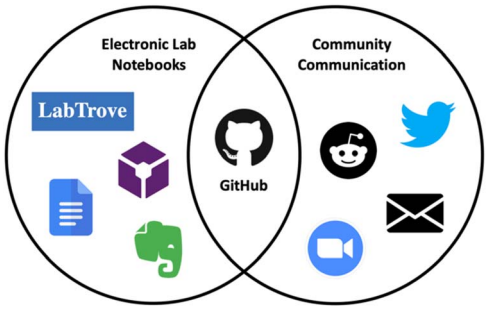
## GitHub as an open electronic laboratory notebook for real-time sharing of knowledge and collaboration

Kymberley R. Scroggie, Klementine J. Burrell-Sander, Peter J. Rutledge and Alice Motion*

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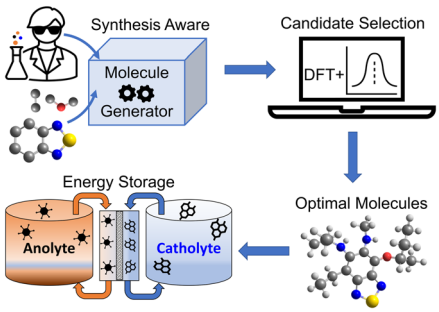
## *In silico* discovery of a new class of anolyte redoxmers for non-aqueous redox flow batteries

Akash Jain, Ilya A. Shkrob, Hieu A. Doan, Lily A. Robertson, Lu Zhang and Rajeev S. Assary*

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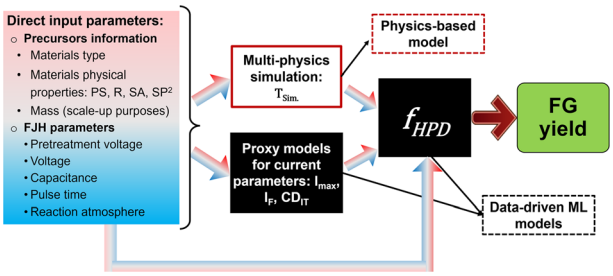
## A scientific machine learning framework to understand flash graphene synthesis

Kianoosh Sattari, Lucas Eddy, Jacob L. Beckham, Kevin M. Wyss, Richard Byfield, Long Qian, James M. Tour* and Jian Lin*

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