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ISSN 2635-098X CODEN DDIIAI 3(2) 223–438 (2024)

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See Michael Levin *et al.*, pp. 249–263. Image reproduced by permission of Patrick McMillen, Levin Lab from *Digital Discovery*, 2024, **3**, 249.

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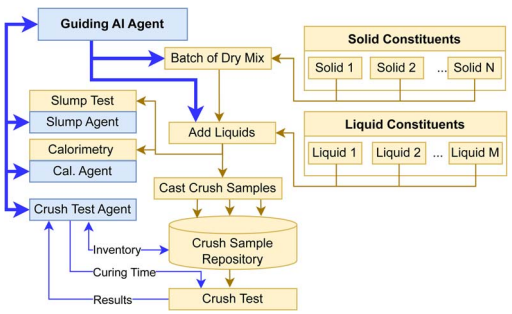
Autonomous cementitious materials formulation platform for critical infrastructure repair

Howie Joress,* Rachel Cook, Austin McDannald, Mark Kozdras, Jason Hattrick-Simpers, Aron Newman and Scott Jones



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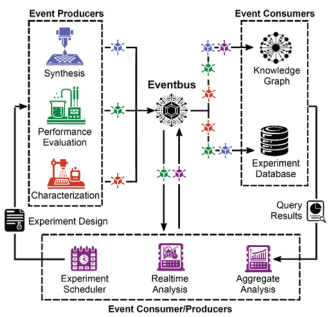
Event-driven data management with cloud computing for extensible materials acceleration platforms

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



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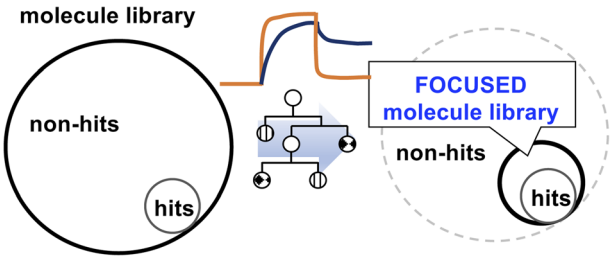
A machine learning approach toward generating the focused molecule library targeting CAG repeat DNA

Qingwen Chen, Takeshi Yamada, Asako Murata, Ayako Sugai, Yasuyuki Matsushita and Kazuhiko Nakatani*



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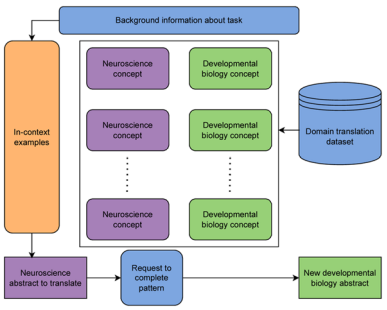
Machine learning for hypothesis generation in biology and medicine: exploring the latent space of neuroscience and developmental bioelectricity

Thomas O'Brien, Joel Stremmel, Léo Pio-Lopez, Patrick McMillen, Cody Rasmussen-Ivey and Michael Levin*



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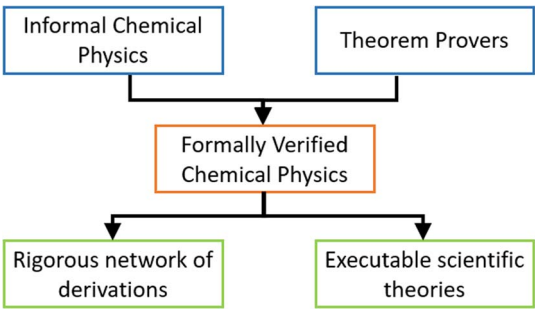
Formalizing chemical physics using the Lean theorem prover

Maxwell P. Bobbin, Samiha Sharlin, Parivash Feyzishendi, An Hong Dang, Catherine M. Wraback and Tyler R. Josephson*



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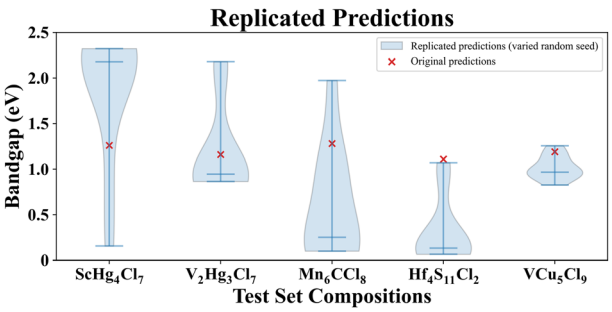
Reproducibility in materials informatics: lessons from 'A general-purpose machine learning framework for predicting properties of inorganic materials'

Daniel Persaud, Logan Ward and Jason Hattrick-Simpers*



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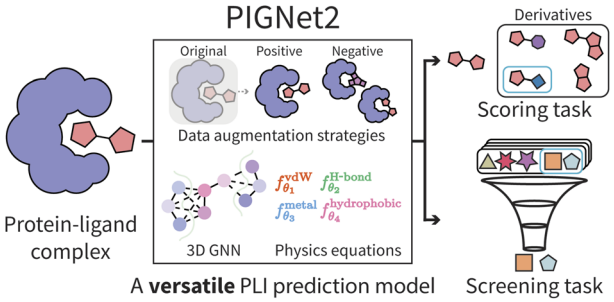

PIGNet2: a versatile deep learning-based protein–ligand interaction prediction model for binding affinity scoring and virtual screening

Seokhyun Moon, Sang-Yeon Hwang, Jaechang Lim and Woo Youn Kim*

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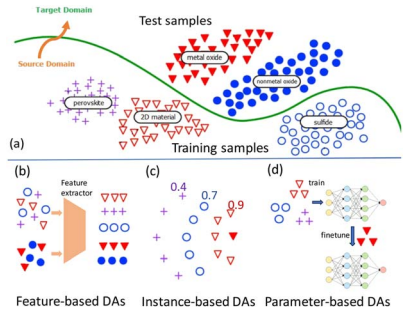

Realistic material property prediction using domain adaptation based machine learning

Jeffrey Hu, David Liu, Nihang Fu and Rongzhi Dong*

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MaScQA: investigating materials science knowledge of large language models

Mohd Zaki, Jayadeva, Mausam and N. M. Anoop Krishnan*

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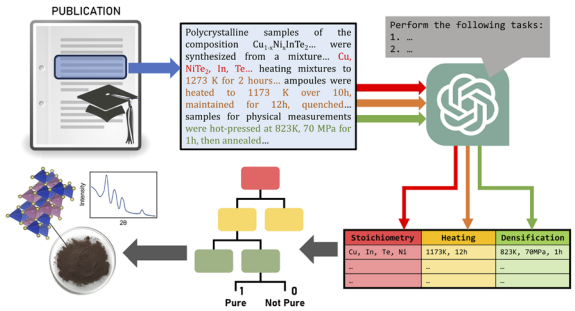

Harnessing GPT-3.5 for text parsing in solid-state synthesis – case study of ternary chalcogenides

Maung Thway, Andre K. Y. Low, Samyak Khetan, Haiwen Dai, Jose Recatala-Gomez, Andy Paul Chen and Kedar Hippalgaonkar*

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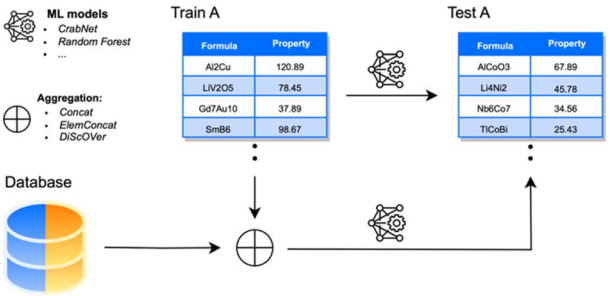
Not as simple as we thought: a rigorous examination of data aggregation in materials informatics

Federico Ottomano, Giovanni De Felice,* Vladimir V. Gusev and Taylor D. Sparks*



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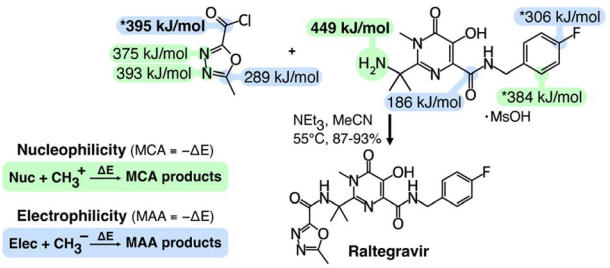
Automated quantum chemistry for estimating nucleophilicity and electrophilicity with applications to retrosynthesis and covalent inhibitors

Nicolai Ree, Andreas H. Göller* and Jan H. Jensen*



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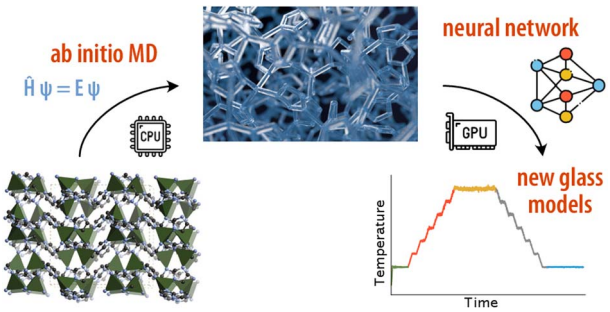
Machine learning interatomic potentials for amorphous zeolitic imidazolate frameworks

Nicolas Castel, Dune André, Connor Edwards, Jack D. Evans* and François-Xavier Coudert*



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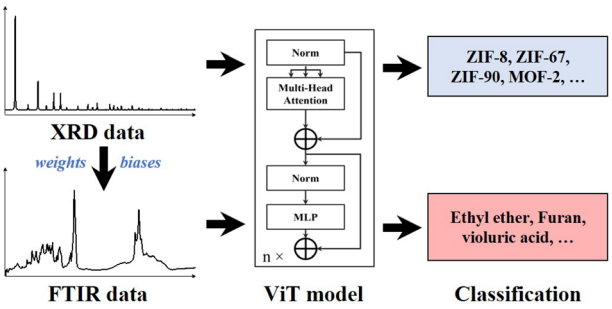
An interpretable and transferrable vision transformer model for rapid materials spectra classification

Zhenru Chen, Yunchao Xie,* Yuchao Wu, Yuyi Lin, Shigetaka Tomiya and Jian Lin*



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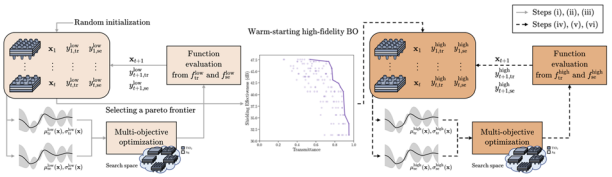

Multi-BOWS: multi-fidelity multi-objective Bayesian optimization with warm starts for nanophotonic structure design

Jungtaek Kim, Mingxuan Li, Yirong Li, Andrés Gómez, Oliver Hinder and Paul W. Leu*

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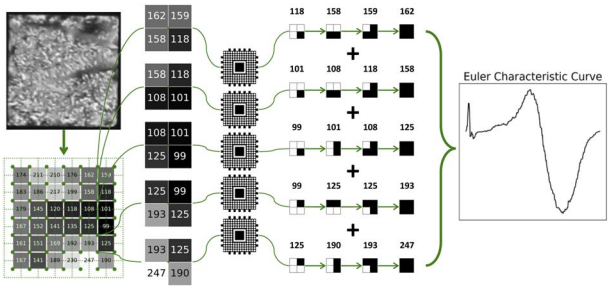

A fast and scalable computational topology framework for the Euler characteristic

Daniel J. Laky and Victor M. Zavala*

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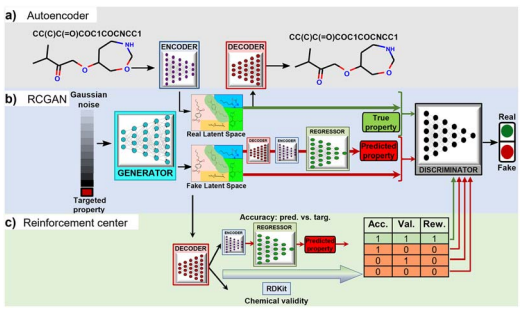

De novo molecule design towards biased properties *via* a deep generative framework and iterative transfer learning

Kianoosh Sattari, Dawei Li, Bhupalee Kalita, Yunchao Xie, Fatemeh Barmaleki Lighvan, Olexandr Isayev and Jian Lin*

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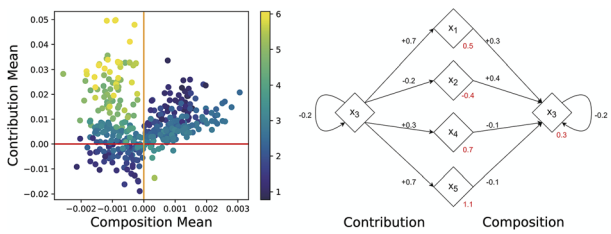

Understanding the importance of individual samples and their effects on materials data using explainable artificial intelligence

Tommy Liu,* Zhi Yang Tho and Amanda S. Barnard

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