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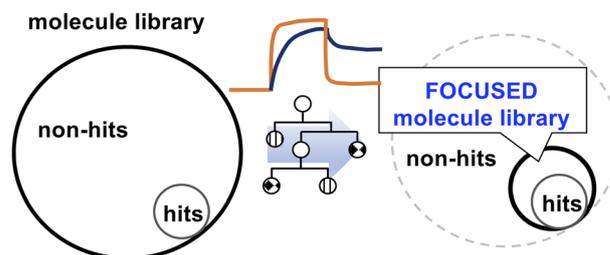
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## COMMUNICATION

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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\*

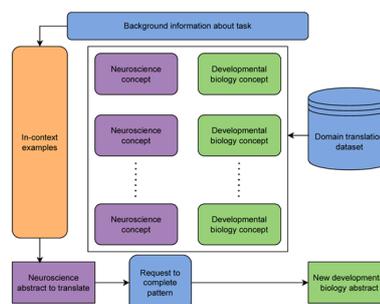


## PAPERS

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

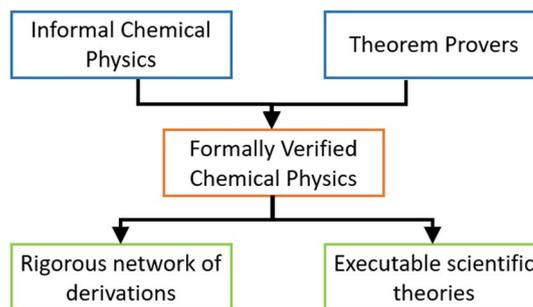
Thomas O'Brien, Joel Stremmel, Léo Pio-Lopez, Patrick McMillen, Cody Rasmussen-Ivey and Michael Levin\*



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**Formalizing chemical physics using the Lean theorem prover**

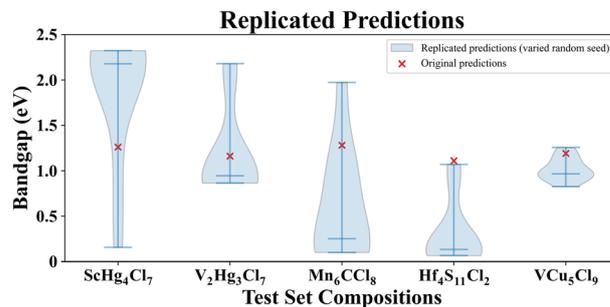
Maxwell P. Bobbin, Samiha Sharlin, Parivash Feyzishendi, An Hong Dang, Catherine M. Wraback and Tyler R. Josephson\*



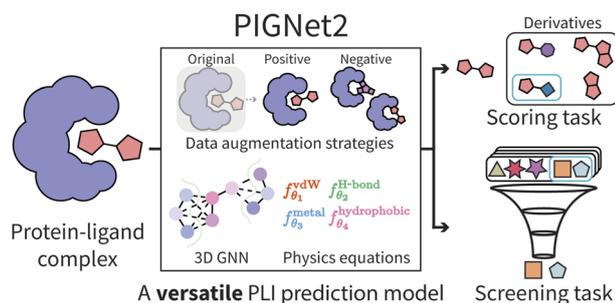
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**Reproducibility in materials informatics: lessons from 'A general-purpose machine learning framework for predicting properties of inorganic materials'**

Daniel Persaud, Logan Ward and Jason Hatrick-Simpers\*



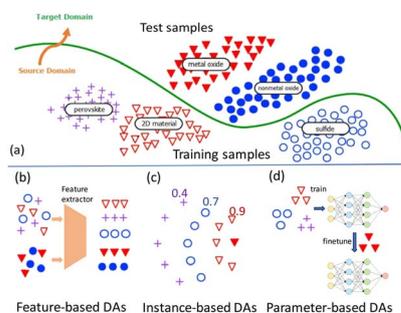
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### PIGNet2: a versatile deep learning-based protein–ligand interaction prediction model for binding affinity scoring and virtual screening

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\*

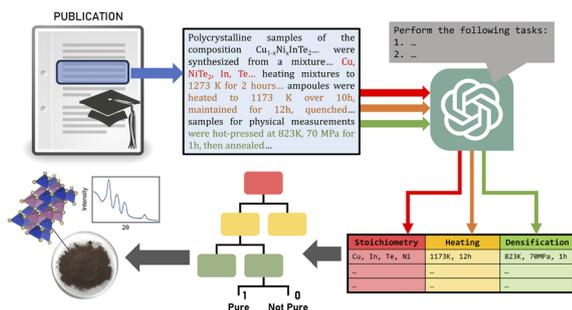
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### MaScQA: investigating materials science knowledge of large language models

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

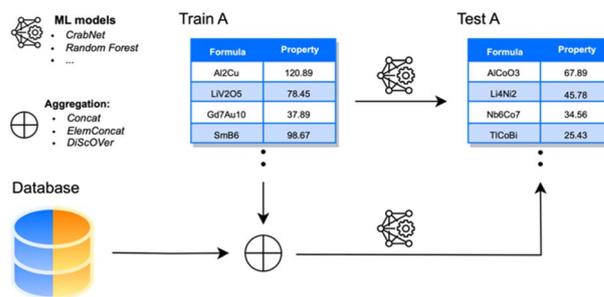
Maung Thway, Andre K. Y. Low, Samyak Khetan, Haiwen Dai, Jose Recatala-Gomez, Andy Paul Chen and Kedar Hippalgaonkar\*



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

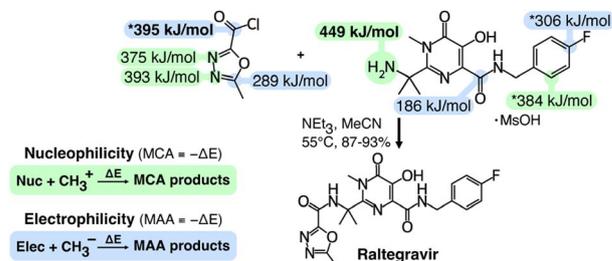
Federico Ottomano, Giovanni De Felice,<sup>\*</sup>  
Vladimir V. Gusev and Taylor D. Sparks<sup>\*</sup>



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

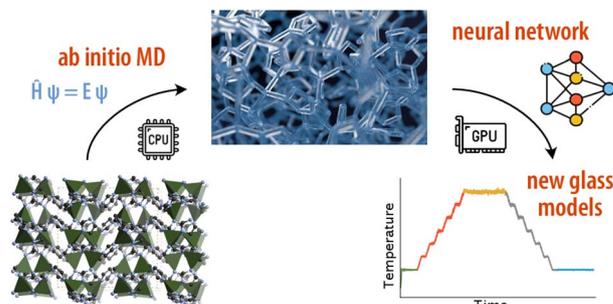
Nicolai Ree, Andreas H. Göller<sup>\*</sup> and Jan H. Jensen<sup>\*</sup>



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## Machine learning interatomic potentials for amorphous zeolitic imidazolate frameworks

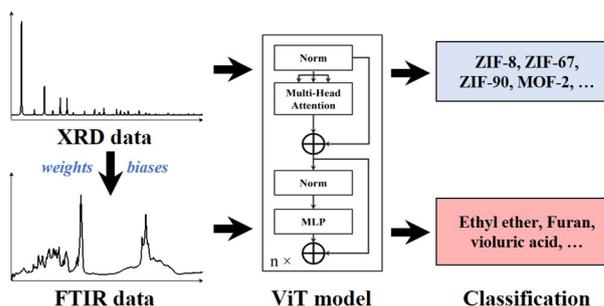
Nicolas Castel, Dune André, Connor Edwards, Jack D. Evans<sup>\*</sup> and François-Xavier Coudert<sup>\*</sup>



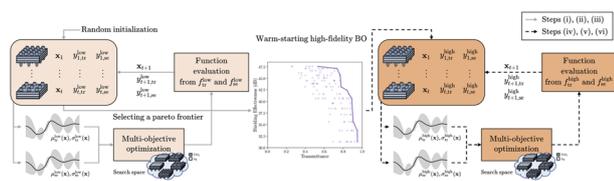
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## An interpretable and transferrable vision transformer model for rapid materials spectra classification

Zhenru Chen, Yunchao Xie,<sup>\*</sup> Yuchao Wu, Yuyi Lin, Shigetaka Tomiya and Jian Lin<sup>\*</sup>



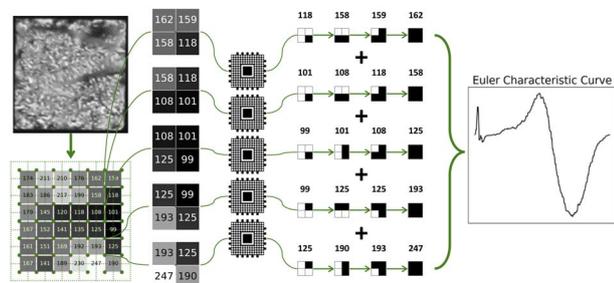
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## Multi-BOWS: multi-fidelity multi-objective Bayesian optimization with warm starts for nanophotonic structure design

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

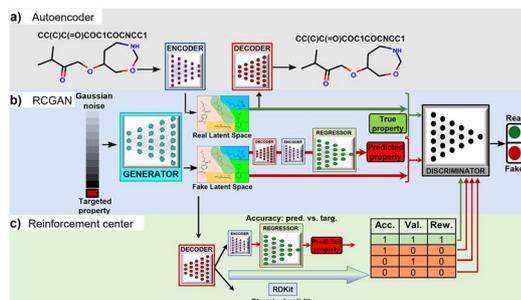
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## A fast and scalable computational topology framework for the Euler characteristic

Daniel J. Laky and Victor M. Zavala\*

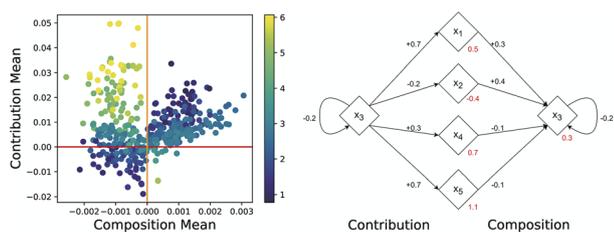
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## De novo molecule design towards biased properties via a deep generative framework and iterative transfer learning

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

