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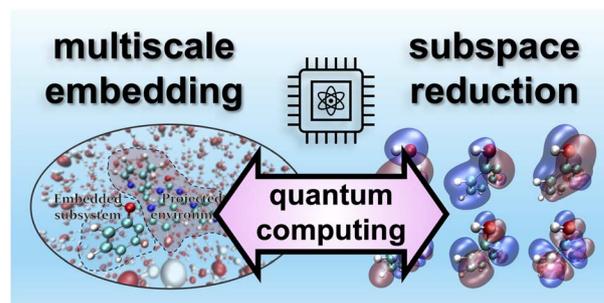
Inside cover
See Ge Lei and Samuel J. Cooper, pp. 3455–3465. Image reproduced by permission of Ge Lei and Samuel J. Cooper from *Digital Discovery*, 2025, 4, 3455. Image created with the use of Google Gemini and Adobe Photoshop Generative Fill.

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Extending quantum computing through subspace, embedding and classical molecular dynamics techniques

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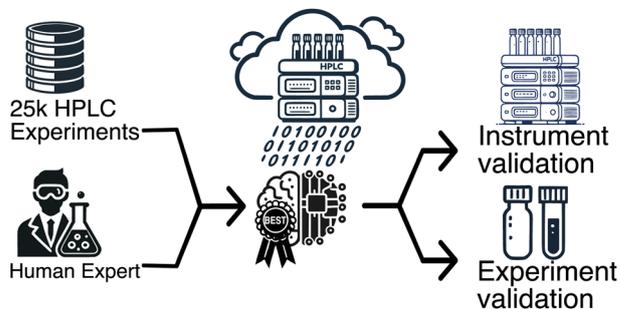


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Machine learning anomaly detection of automated HPLC experiments in the cloud laboratory

Filipp Gusev, Benjamin C. Kline, Ryan Quinn, Anqin Xu, Ben Smith, Brian Frezza and Olexandr Isayev*



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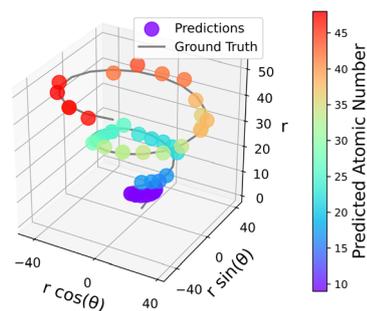


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Do Llamas understand the periodic table?

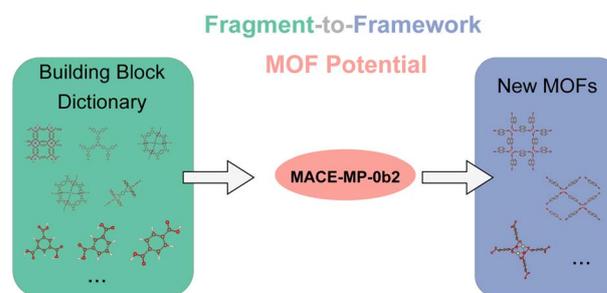
Ge Lei* and Samuel J. Cooper



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FFLAME: a fragment-to-framework learning approach for MOF potentials

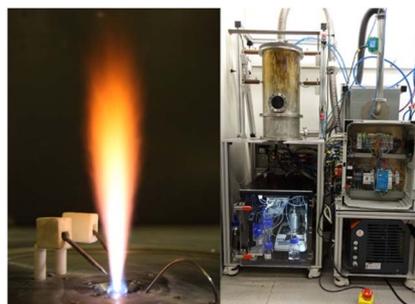
Xiaoqi Zhang, Yutao Li, Xin Jin and Berend Smit*



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An automated platform for “on-demand” high-speed catalyst synthesis by flame spray pyrolysis

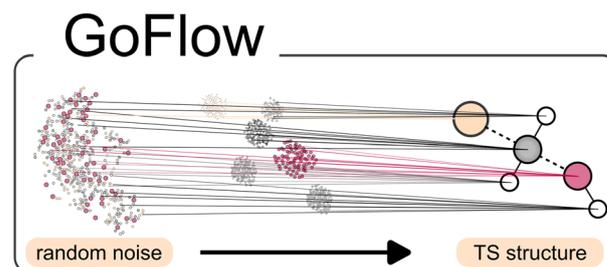
Konstantin M. Engel, Patrik O. Willi, Robert N. Grass and Wendelin J. Stark*



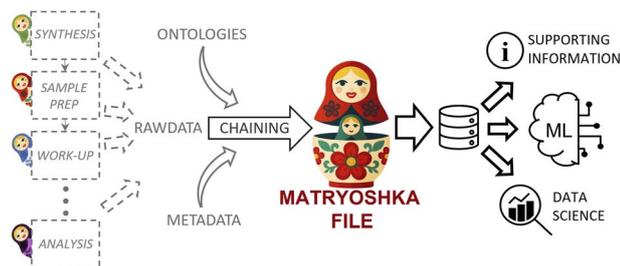
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GoFlow: efficient transition state geometry prediction with flow matching and E(3)-equivariant neural networks

Leonard Galustian, Konstantin Mark, Johannes Karwounopoulos, Maximilian P.-P. Kovar and Esther Heid*



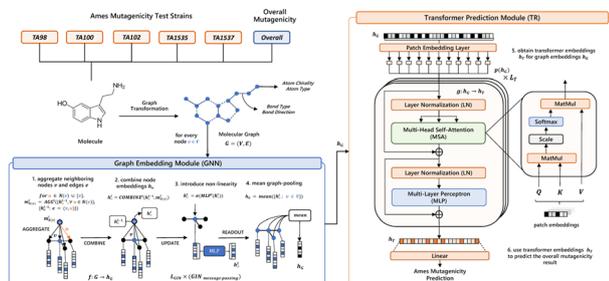
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A FAIR research data infrastructure for high-throughput digital chemistry

Alice Gauthier, Laure Vancauwenberghe, Jean-Charles Cousty,* Cyril Matthey-Doret, Robin Franken, Sabine Maennel, Pascal Miéville and Oksana Riba Grognez

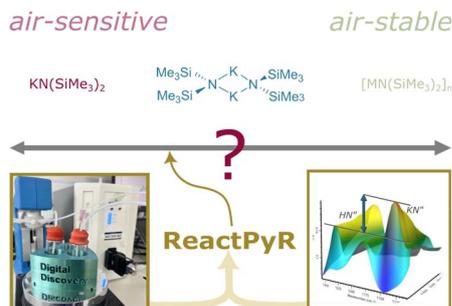
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Advancing mutagenicity predictions in drug discovery with an explainable few-shot deep learning framework

Luis H. M. Torres,* Sofia M. da Silva, Joel P. Arrais, Catarina Pimentel and Bernardete Ribeiro

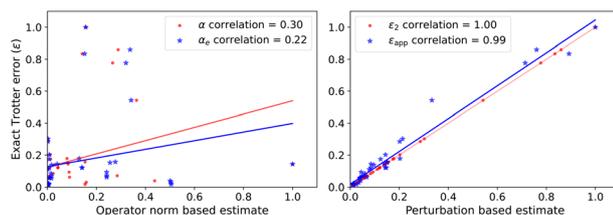
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ReactPyR: a python workflow for ReactIR allows for quantification of the stability of sensitive compounds in air

Nicola L. Bell,* Emanuele Berardi, Marina Gladkikh, Richard Drummond Turnbull and Freya Turton

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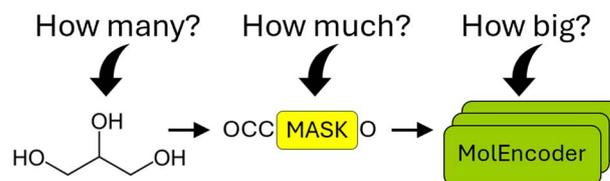


Estimating Trotter approximation errors to optimize Hamiltonian partitioning for lower eigenvalue errors

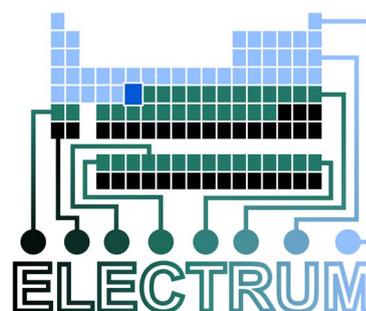
Shashank G. Mehendale, Luis A. Martínez-Martínez, Pratham Divakar Kamath and Artur F. Izmaylov*



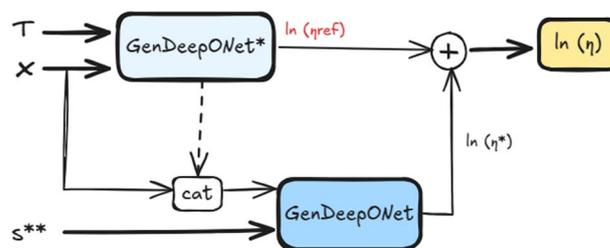
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MolEncoder: towards optimal masked language modeling for moleculesFabian P. Krüger,^{*} Nicklas Österbacka, Mikhail Kabeshov, Ola Engkvist and Igor Tetko

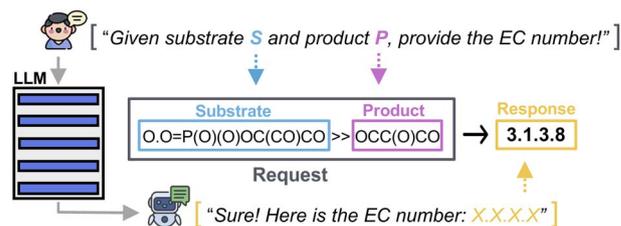
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ELECTRUM: an electron configuration-based universal metal fingerprint for transition metal compoundsMarkus Orsi^{*} and Angelo Frei^{*}

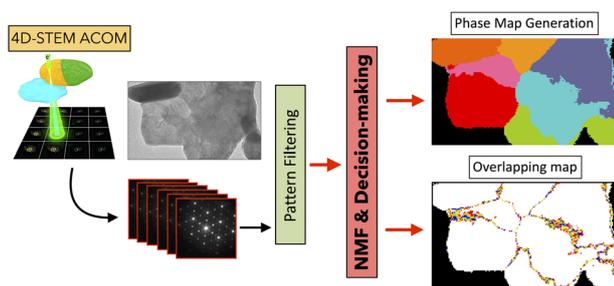
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Generalized DeepONets for viscosity prediction using learned entropy scaling referencesMaximilian Fleck,^{*} Marcelle B. M. Spera, Samir Darouich, Timo Klenk and Niels Hansen^{*}

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Leveraging large language models for enzymatic reaction prediction and characterizationLorenzo Di Fruscia and Jana M. Weber^{*}

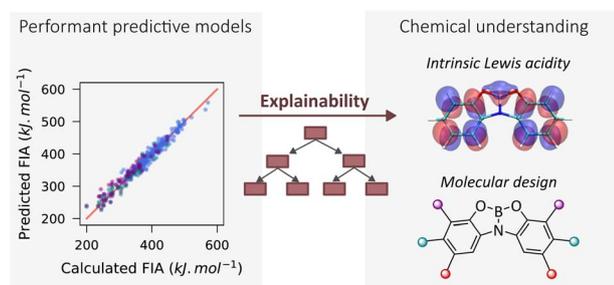
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Unsupervised multi-clustering and decision-making strategies for 4D-STEM orientation mapping

Junhao Cao, Nicolas Folastre, Gozde Oney, Edgar Rauch, Stavros Nicolopoulos, Partha Pratim Das and Arnaud Demortière*

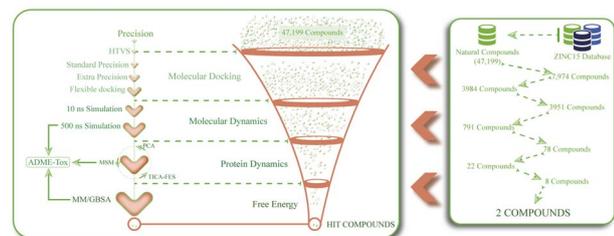
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Constructing and explaining machine learning models for the exploration and design of boron-based Lewis acids

Juliette Fenogli*, Laurence Grimaud* and Rodolphe Vuilleumier*

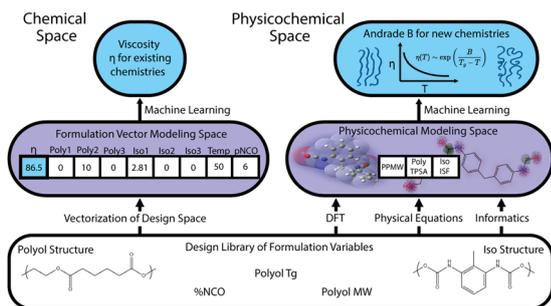
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Database mining of ZINC15 natural compounds reveals potential thyroid receptor β agonists for NAFLD management: an *in silico* study

Ahmet Buğra Ortaakarsu*, Michel Hosny, Mansour Sobeh and Mohamed A. O. Abdelfattah

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Machine learning of polyurethane prepolymer viscosity: a comparison of chemical and physicochemical approaches

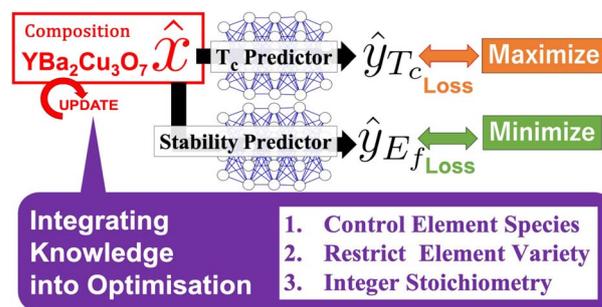
Joseph A. Pugar, Calvin Gang, Isabelle Millan, Karl Haider and Newell R. Washburn*



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A straightforward gradient-based approach for designing superconductors with high critical temperature: exploiting domain knowledge via adaptive constraints

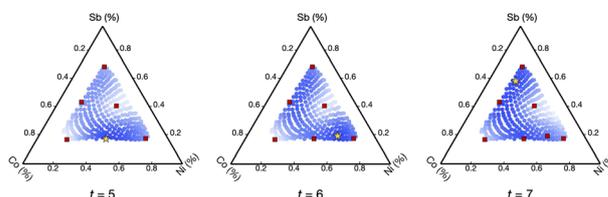
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Active learning path-dependent properties using a cloud-based materials acceleration platform

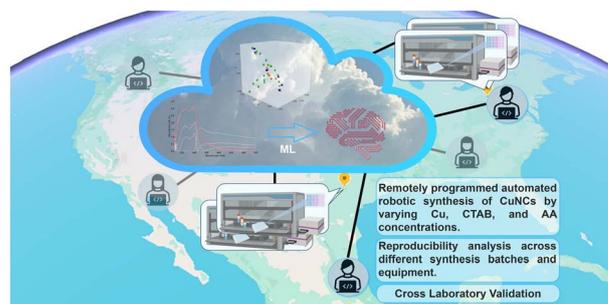
Dan Guevarra, Michael J. Statt,* Kostiantyn Popovich, Brian A. Rohr,* John M. Gregoire, Kevin Tran, Santosh K. Suram, Joel A. Haber* and Willie Neiswanger*



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Cross-laboratory validation of machine learning models for copper nanocluster synthesis using cloud-based automated platforms

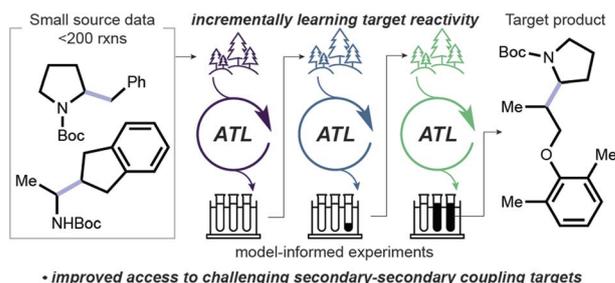
Ricardo Montoya-Gonzalez, Rosa de Guadalupe González-Huerta, Martha Leticia Hernández-Pichardo and Subha R. Das*



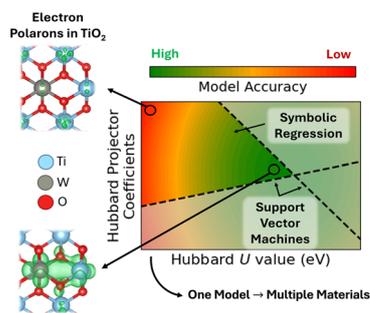
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Prospective active transfer learning on the formal coupling of amines and carboxylic acids to form secondary alkyl bonds

Eunjae Shim, Ambuj Tewari, Paul M. Zimmerman* and Tim Cernak*



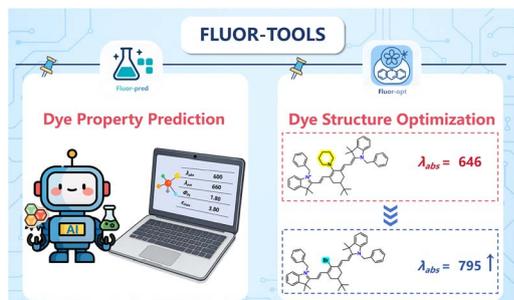
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Machine learning generalised DFT+*U* projectors in a numerical atom-centred orbital framework

Amit Chaudhari, Kushagra Agrawal and Andrew J. Logsdail*

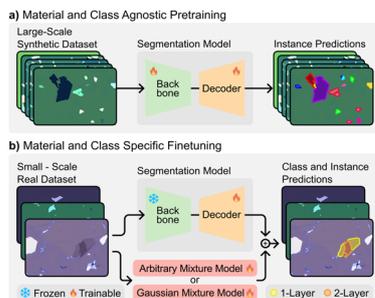
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Fluor-tools: an integrated platform for dye property prediction and structure optimization

Wenxiang Song, Yuyang Zhang, Le Xiong, Xinmin Li, Jingwei Zhang, Guixia Liu, Weihua Li, Youjun Yang* and Yun Tang*

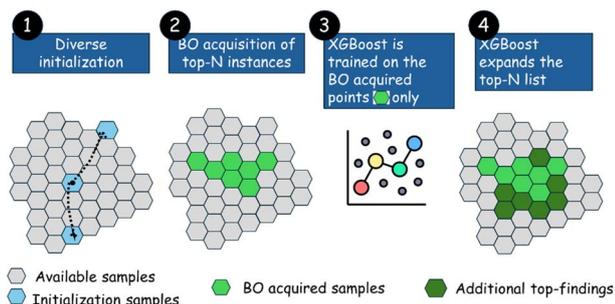
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MaskTerial: a foundation model for automated 2D material flake detection

Jan-Lucas Uslu,* Alexey Nekrasov, Alexander Hermans, Bernd Beschoten, Bastian Leibe, Lutz Waldecker and Christoph Stampfer

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Navigating materials design spaces with efficient Bayesian optimization: a case study in functionalized nanoporous materials

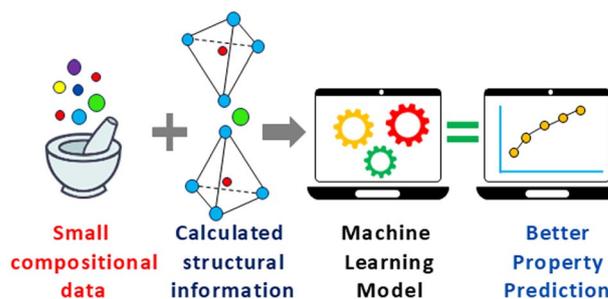
Panagiotis Krokidas,* Vassilis Gkatsis, John Theocharis and George Giannakopoulos



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An improved machine learning strategy using structural features to predict the glass transition temperature of oxide glasses

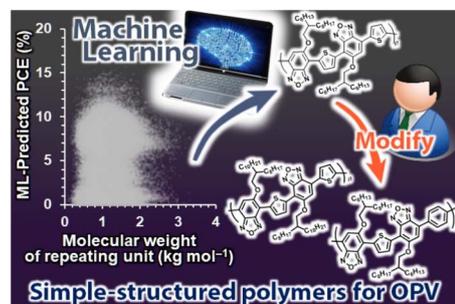
Satwinder Singh Danewalia* and Kulvir Singh



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Design of simple-structured conjugated polymers for organic solar cells by machine learning-assisted structural modification and experimental validation

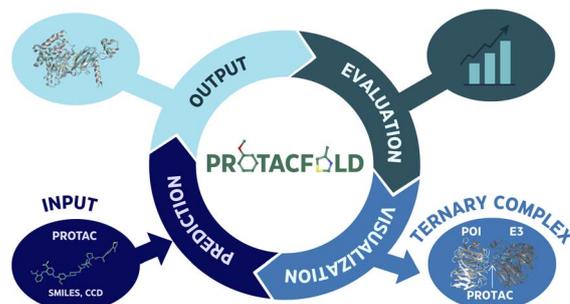
Shogo Tadokoro, Ryosuke Kamimura, Fumitaka Ishiwari and Akinori Saeki*



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Predicting PROTAC-mediated ternary complexes with AlphaFold3 and Boltz-1

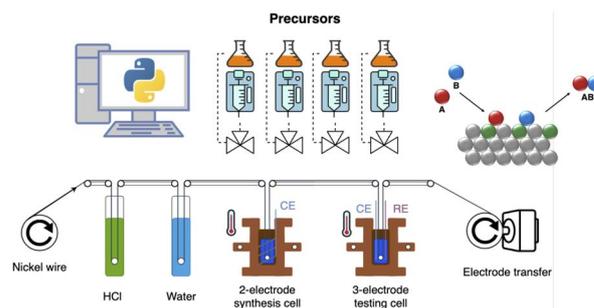
Nils Dunlop, Francisco Erazo, Farzaneh Jalalypour and Rocío Mercado*



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CatBot – a high-throughput catalyst synthesis and testing system with roll to roll transfer

Paolo Vincenzo Freiesleben de Blasio,* Rune Kruger, Nis Fisker-Bødker, Jin Hyun Chang and Christodoulos Chatzichristodoulou



PAPERS

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**Multi-modal contrastive learning for chemical structure elucidation with VibraCLIP**

Pau Rocabert-Oriols, Camilla Lo Conte, Núria López and Javier Heras-Domingo*

CORRECTION

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Correction: Beyond training data: how elemental features enhance ML-based formation energy predictions

Hamed Mahdavi,* Vasant Honavar and Dane Morgan

