Enhancing Materials Property Prediction: A Multimodal Learning via Image Mapping of Material Compositions

Yu Yeyong [a], Wu Xing [a,c], Zhang Huiran[a,c], Qian Quan [a, b, c,*]

[a.] School of Computer Engineering and Science, Shanghai University

[b.] Materials Genome Institute, Shanghai University, Shanghai

[c.] Zhejiang Laboratory, Hangzhou **Email: qqian@shu.edu.cn**

上海大学 SHANGHAI UNIVERSITY

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"Unlocking the AI Future of Materials Science"

Introduction

- **Complex material datasets** challenge machine learning due to sparse features.
- **Composition crucial**: composition proportions overlooked.
- **Compositional features present**: Atomic info missing.
- **Image mapping**: Using XenonPy expand 58 elemental points, 406 extended dimensions.
- **Grayscale images** for CNN extraction.

Methods

Densification and Prediction: Atomic features for 2D grayscale images; MCVN predicts steel properties, classifies amorphous alloys. [See Figure A]

- **Expert-based visualization**: Enhances compositional features in material ML tasks.
- **Multimodal deep-network model**: Integrates visualization images & raw features, improves accuracy. [See Figure B]

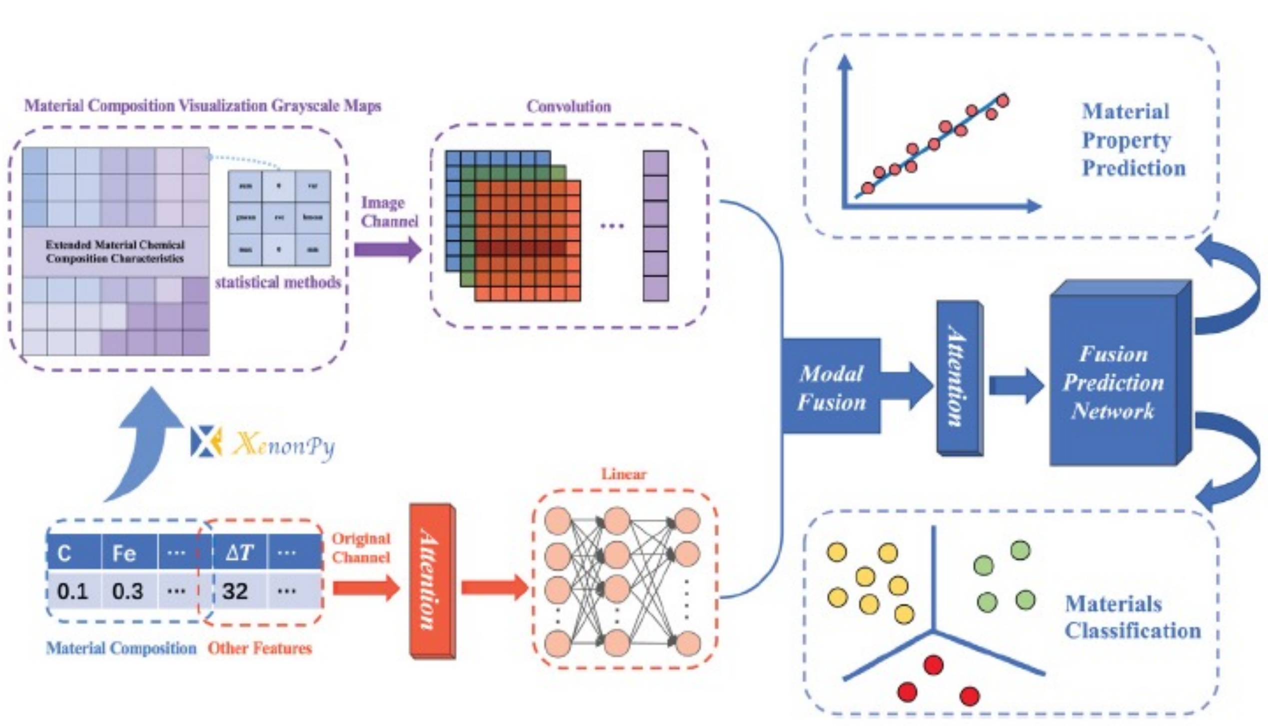


Figure A. Better utilization of composition for material property prediction using the MCVN.

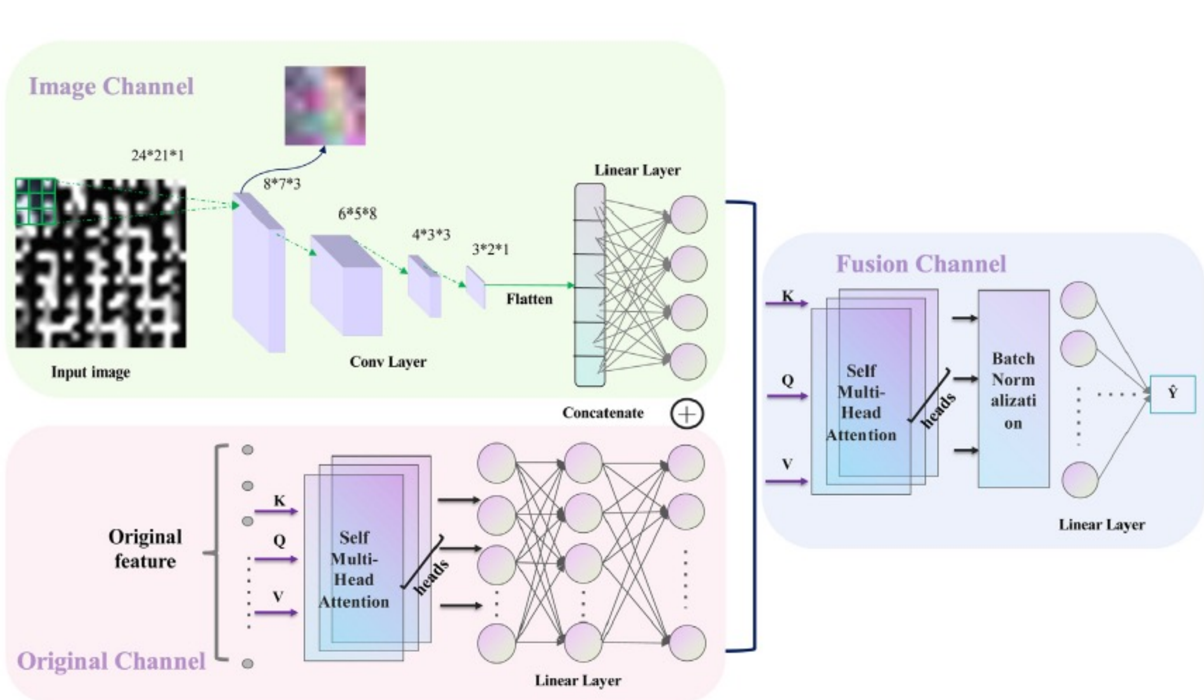
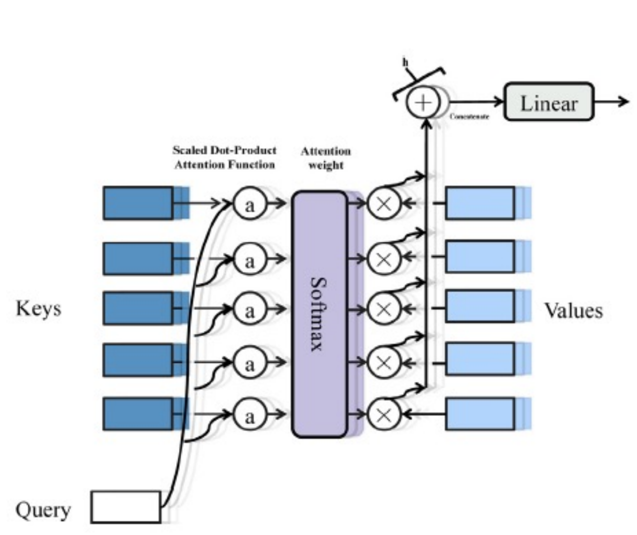
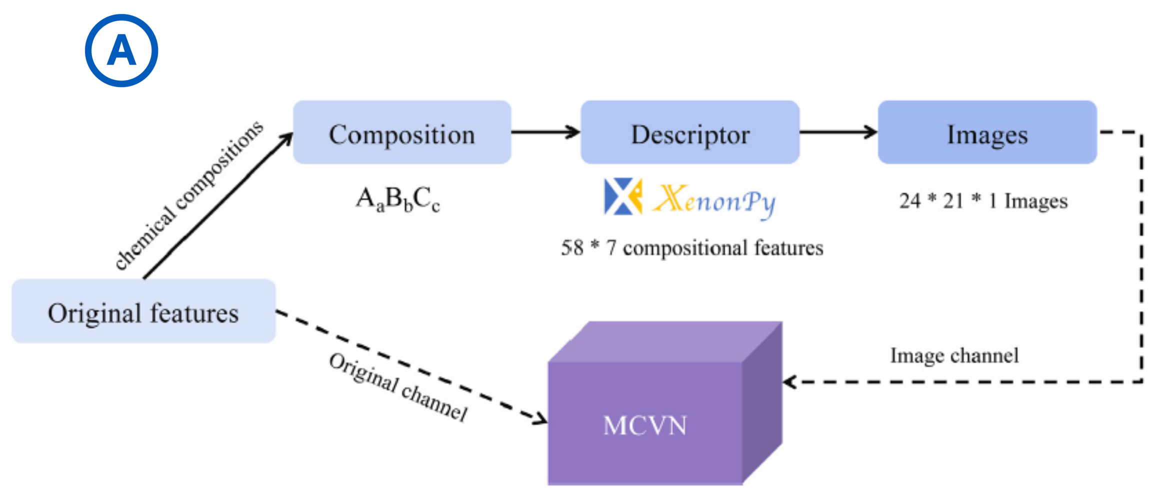


Figure B. Material composition visualization network architecture.

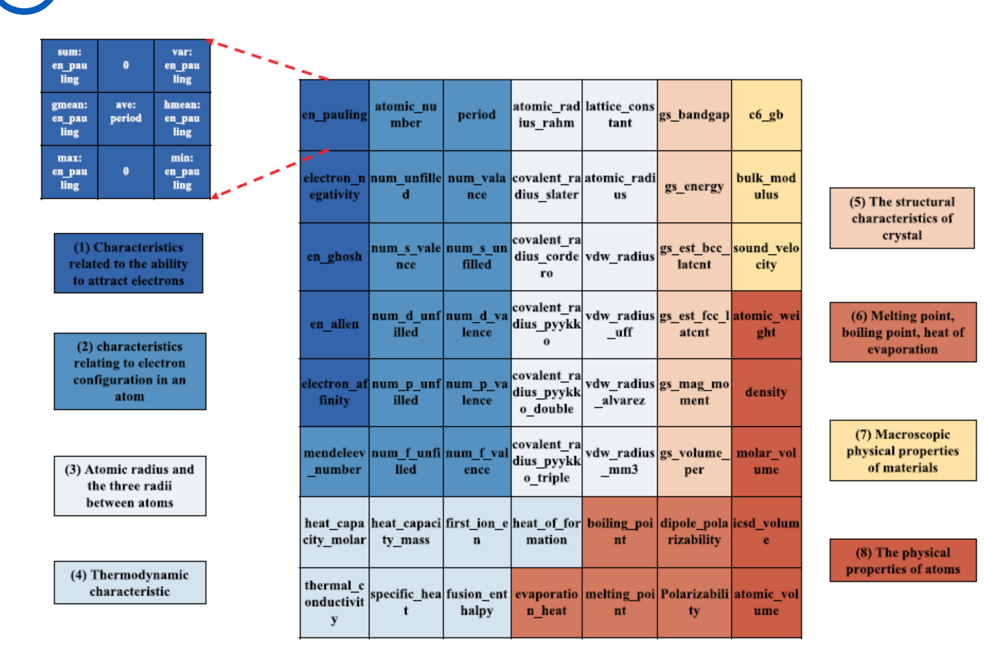


Self-attention Mechanism: Reduces external info reliance, captures internal relevance effectively.

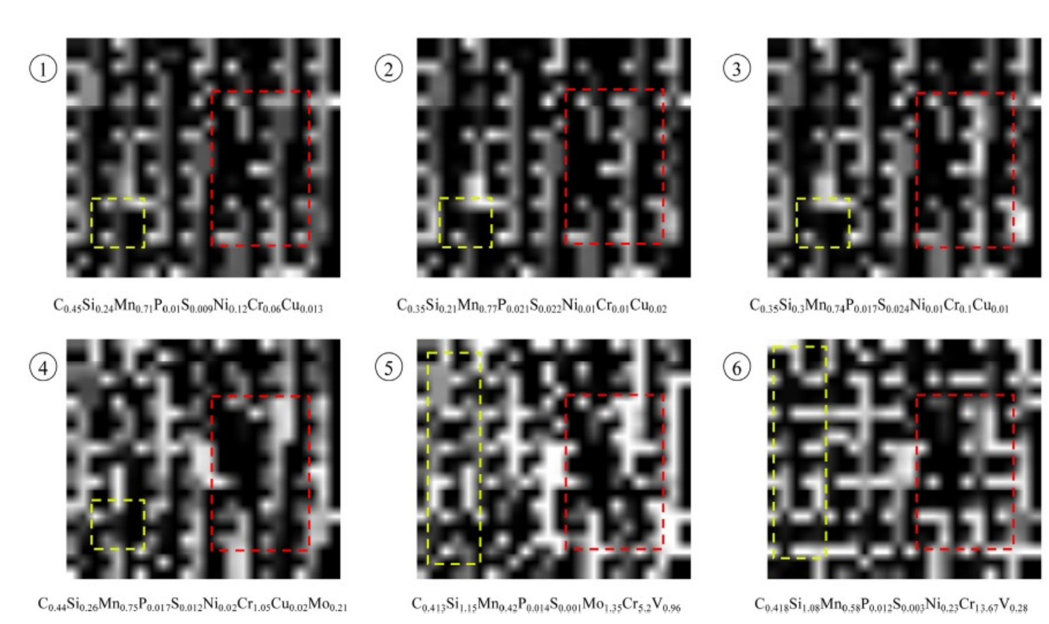
Modal Translation



Process Flow: Feature Enhancement with Xenonpy.



Arrangement: Template of compositional features.



Grayscale Image: Element-level description of features

Results

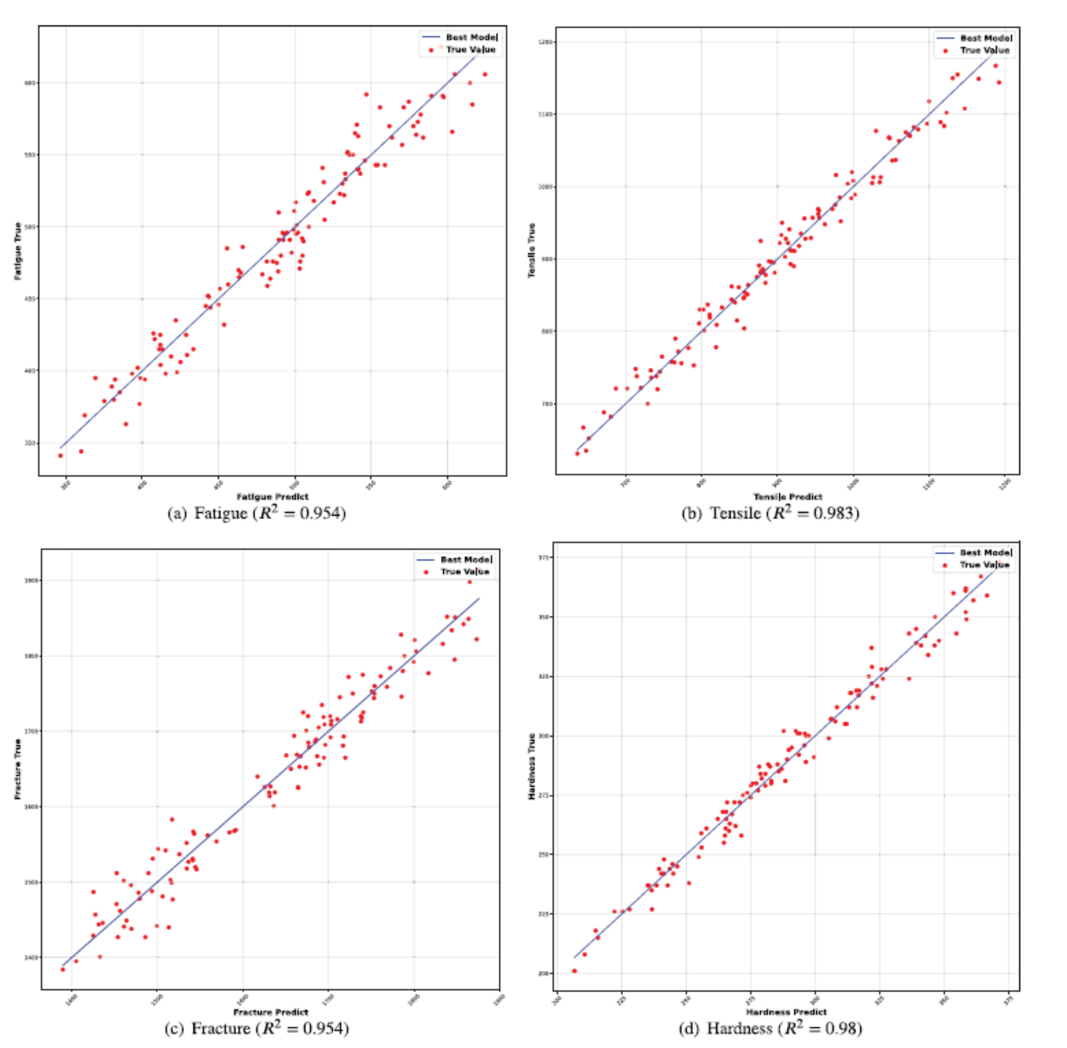
Classification Task

Algorithm	Category		Precision	Recall	F1-score	Support
RF (Breiman, 2015)	BMG	*O*	0.83	**0.94**	0.87	208
		E	0.72	0.93	0.82	
		E&P	0.77	0.92	0.84	
	RMG	*O*	0.82	0.94	0.87	1241
		E	0.83	0.92	0.87	
		E&P	0.81	0.92	0.86	
	CRA	*O*	0.86	0.52	0.65	510
		E	0.88	0.54	0.67	
		E&P	0.83	0.50	0.62	
XGBoost (Chen and Guestrin, 2016)	BMG	*O*	0.92	0.85	0.89	208
		E	0.92	0.87	0.90	
		E&P	0.92	0.80	0.86	
	RMG	*O*	0.83	0.95	0.89	1241
		E	0.86	0.94	0.90	
		E&P	0.81	**0.95**	0.87	
	CRA	*O*	0.83	0.57	0.68	510
		E	0.84	0.67	0.75	
		E&P	0.83	0.54	0.66	
Attention Network (Vaswani et al., 2017)	BMG	*O*	0.842	0.875	0.858	208
		E	0.895	0.860	0.877	
		E&P	0.899	0.861	0.879	
	RMG	*O*	0.871	0.905	0.888	1241
		E	0.890	0.905	0.898	
		E&P	0.885	0.913	0.899	
	CRA	*O*	0.786	0.583	0.684	510
		E	0.794	0.562	0.678	
		E&P	0.806	0.596	0.70	
edRVFL_N (Shi et al., 2022)	BMG	*O*	0.936	0.567	0.706	208
		E	**0.967**	0.860	0.910	
		E&P	0.937	0.581	0.718	
	RMG	*O*	0.770	0.923	0.840	1241
		E	0.847	0.930	0.887	
		E&P	0.785	0.930	0.851	
	CRA	*O*	0.742	0.503	0.600	510
		E	0.798	0.643	0.712	
		E&P	0.777	0.547	0.642	
MCVN	BMG		0.931	0.904	**0.917**	208
	RMG		**0.901**	0.941	**0.921**	1241
	CRA		**0.861**	**0.778**	**0.818**	510

Unbalanced amorphous alloy dataset: Increased avg. *Recall* (CRA small-class) from 0.58 to 0.78.

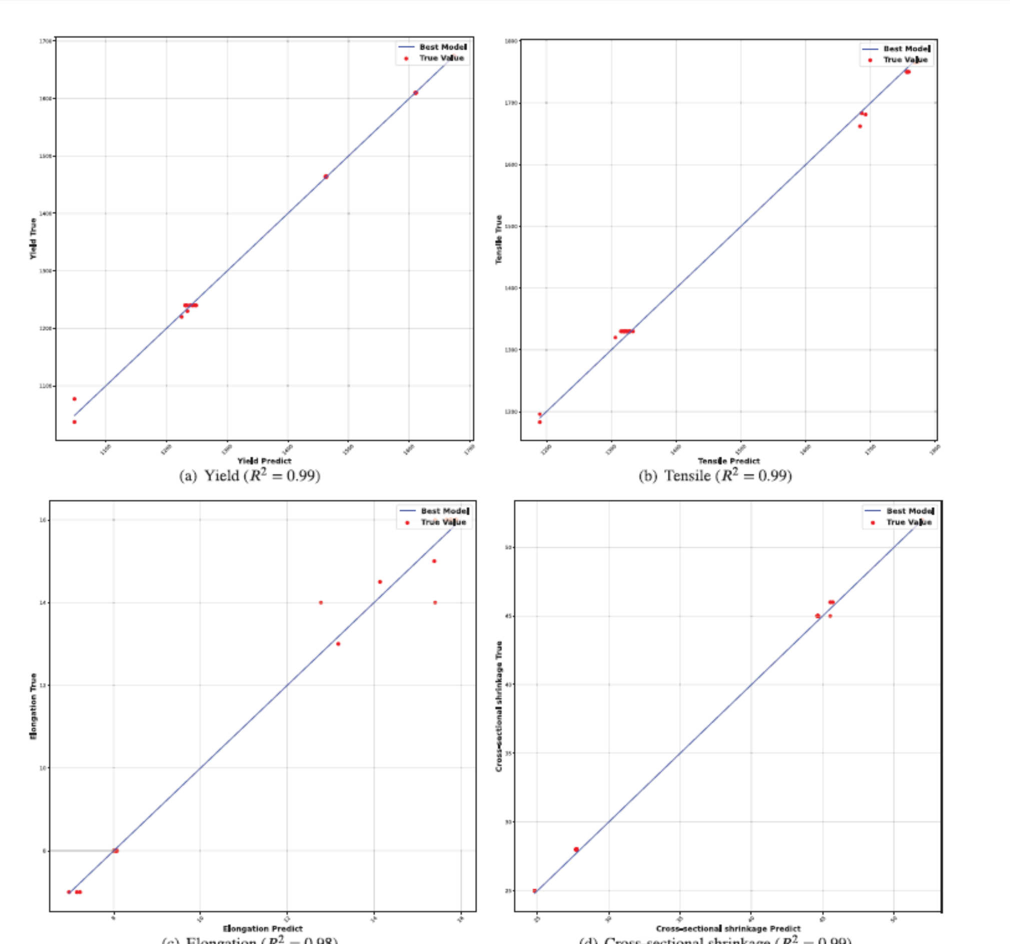
Regression Task

Target	MCVN	Attention Network (Vaswani et al., 2017)			edRVFL_N (Shi et al., 2022)			Ridge (Bottou, 2010)			SVR (Chang and Lin, 2011)			RF (Breiman, 2015)			XGBoost (Chen and Guestrin, 2016)		
		O	*E*	*E&P*	*O*	*E*	*E&P*	*O*	*E*	*E&P*	*O*	*E*	*E&P*	*O*	*E*	*E&P*	*O*	*E*	*E&P*
Fatigue	**0.954**	0.937	0.926	0.939	0.915	0.949	0.913	0.909	0.913	0.908	0.89	0.780	0.882	0.903	0.886	0.904	0.920	0.931	0.921
Tensile	**0.983**	0.966	0.958	0.968	0.936	0.973	0.952	0.939	0.945	0.938	0.925	0.785	0.916	0.919	0.919	0.90	0.942	0.951	0.928
Fracture	**0.954**	0.937	0.942	0.947	0.869	0.920	0.864	0.894	0.915	0.905	0.905	0.859	0.907	0.913	0.941	0.929	0.925	0.930	0.936
Hardness	**0.980**	0.965	0.954	0.968	0.923	0.960	0.926	0.927	0.940	0.929	0.907	0.783	0.899	0.927	0.934	0.904	0.935	0.948	0.931



NIMS's steel dataset: 4% R^2 improvement (0.92 avg. R^2)

Target	MCVN	Attention Network (Vaswani et al., 2017)			edRVFL_N (Shi et al., 2022)			Ridge (Bottou, 2010)			SVR (Chang and Lin, 2011)			RF (Breiman, 2015)			XGBoost (Chen and Guestrin, 2016)		
		O	*E*	*E&P*	*O*	*E*	*E&P*	*O*	*E*	*E&P*	*O*	*E*	*E&P*	*O*	*E*	*E&P*	*O*	*E*	*E&P*
Yield	**0.974**	0.932	0.912	0.938	0.928	0.947	0.940	0.923	0.949	0.928	0.891	0.899	0.880	0.926	0.947	0.944	0.908	0.926	0.922
Tensile	**0.98**	0.942	0.924	0.956	0.957	0.970	0.956	0.944	0.959	0.942	0.918	0.905	0.878	0.94	0.958	0.933	0.915	0.948	0.95
Elongation	**0.943**	0.912	0.897	0.927	0.843	0.869	0.872	0.882	0.77	0.858	0.875	0.858	0.859	0.859	0.860	0.830	0.823	0.814	0.793
Cross-sectional shrinkage	**0.835**	0.638	0.593	0.723	0.729	0.701	0.755	0.624	0.596	0.654	0.544	0.617	0.582	0.668	0.556	0.658	0.656	0.411	0.605



SRIM's steel dataset: $R^2 = 0.835$ on EL (vs 0.64 avg. R^2).

Conclusion

This approach enhances model performances on small sparse matrix samples by expanding material composition data, offering a universal paradigm for predicting material properties.

- **Feature Enhancement:** Densifies sparse composition, boosts generalization.
- **Modal Translation:** XenonPy, element-level features, multimodal grayscale dataset.
- **Multimodal Learning:** MCVN enhances material property predictions.

Reference

1. **Better utilization of materials' compositions for predicting their properties: Material composition visualization network[J]. Engineering Applications of Artificial Intelligence**
2. **FTAP: Feature transferring autonomous machine learning pipeline[J]. Information Sciences**

Organizer

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