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A practical inverse design approach for high-entropy catalysts using generative AI

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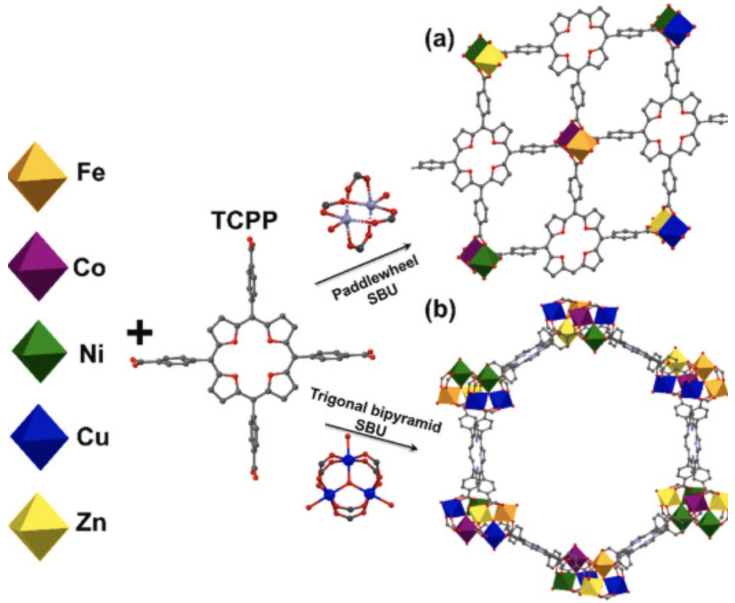
High-entropy catalysts

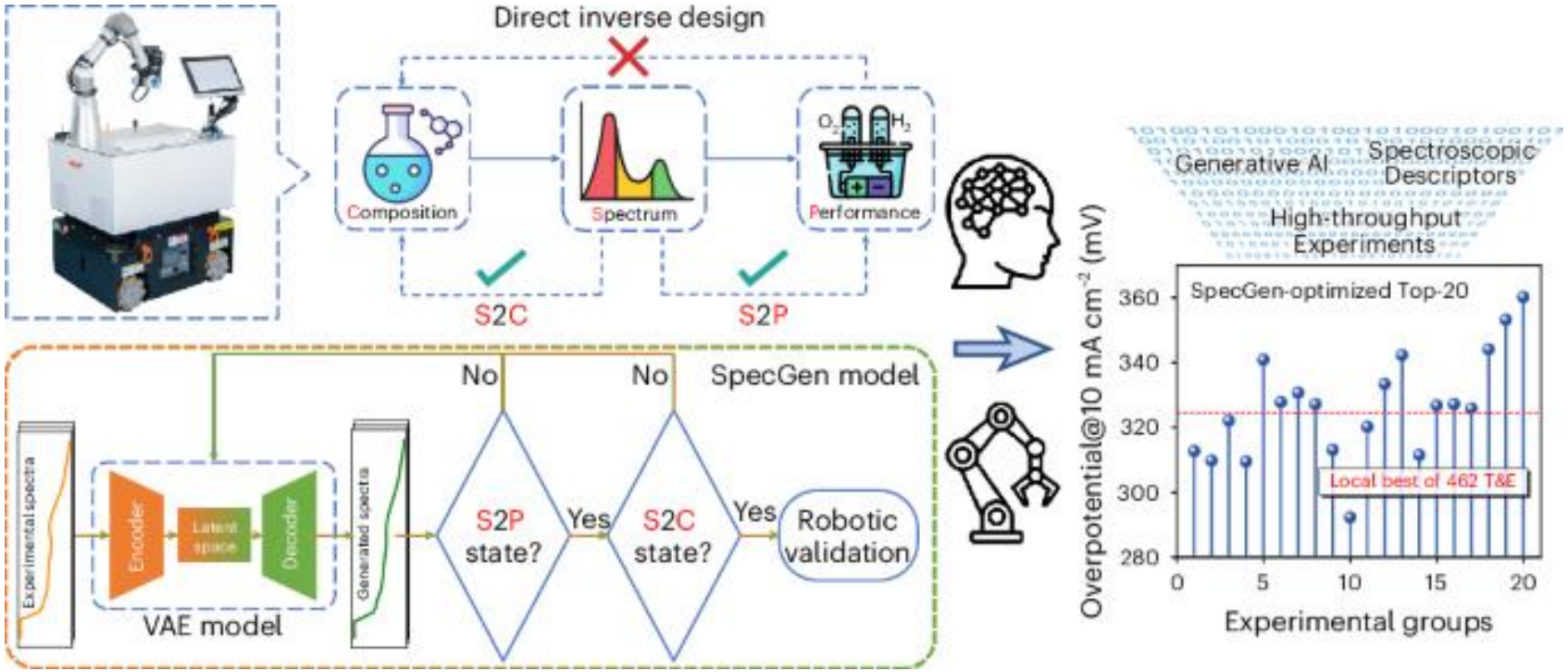
electrocatalytic or thermocatalytic systems that utilize high-entropy materials as catalysts

- **The compositional space of high-entropy materials is nearly infinite**
- **The composition–structure–performance relationship is highly complex**
- **Inverse design remains challenging**
- **Lack of high-throughput experimental validation tools**

In this research

- **Use spectroscopic descriptors as a bridge variable**
- **Establish an AI–robotics closed-loop platform**
- **Accelerate the discovery of high-performance OER catalysts**





AI-Chemist

The system uses integrated robotic arms and automated modules, linked to a cloud server, to enable fully remote catalyst preparation and analysis.

SepcGen

VAE: extracting and generating spectral features from spectroscopic descriptors

S2P model: predicting catalytic overpotential

S2C model: predicting metal composition

AI-Chemist

Autonomous experiment platform validates the catalysts with suggested composition

Predicted composition of those 20 virtual spectra

Synthesized and characterized 624 catalyst samples

Original dataset

Model training

S2C Model

Model training

S2P Model

20 best virtual spectra

Real spectra

VAE

Generated 10 million virtual spectra

virtual spectra

AI-Chemist

Dispensing

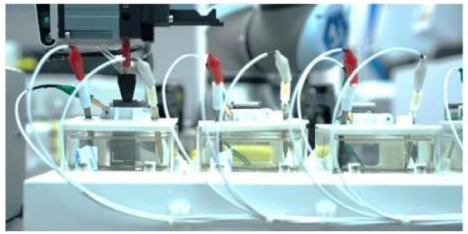
Magnetic stirring

Centrifugation

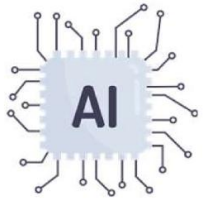
Solid-liquid separation

Drying

UV-Vis-NIR



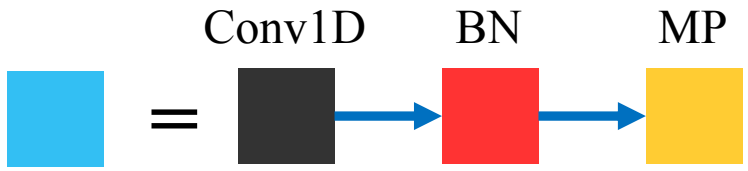
Catalytic performance test

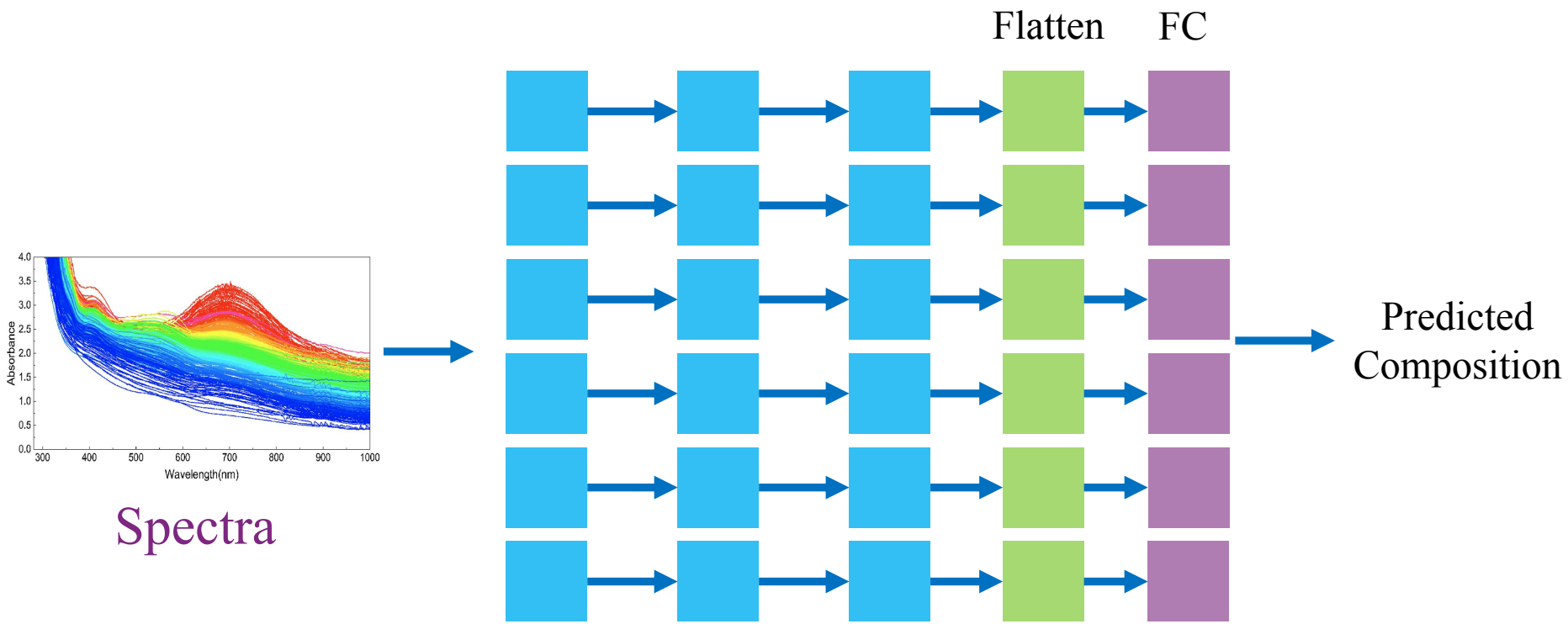


SpecGen prediction

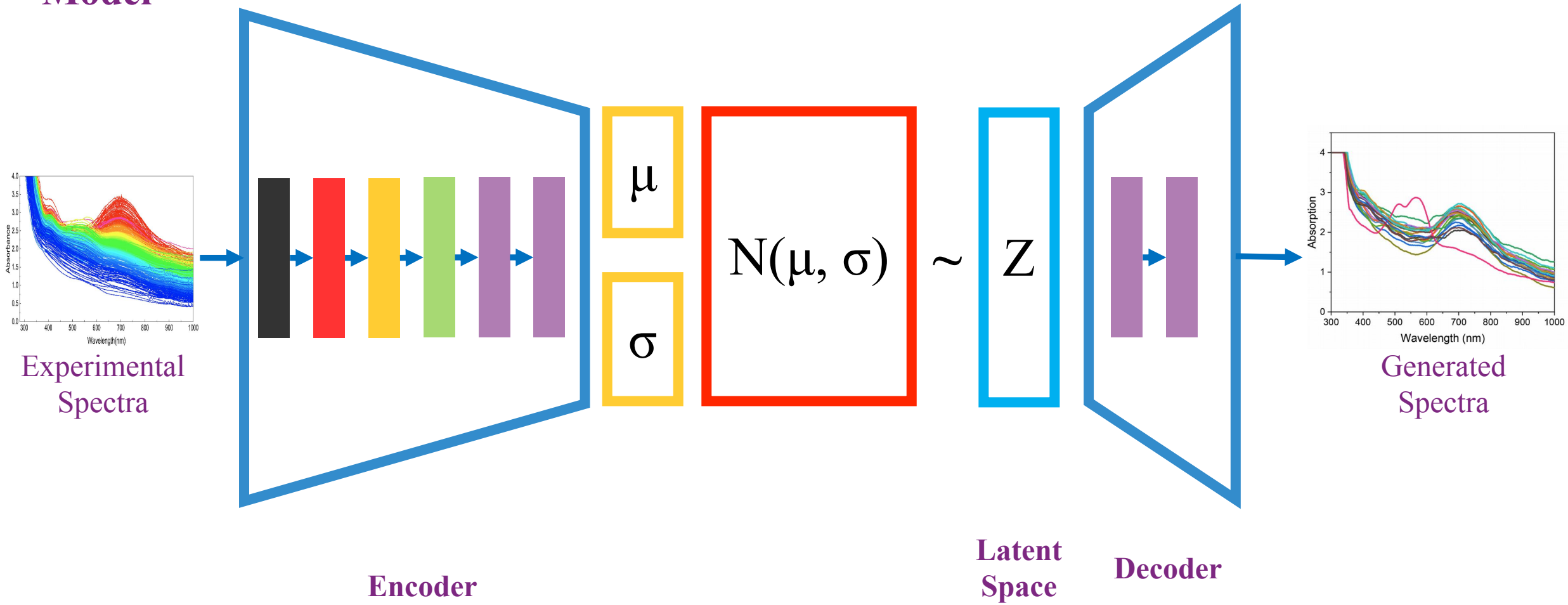
Characterization and performance testing from approximately 20 hours to only 78 minutes per sample.

S2C Model


Conv1D
BN
MP

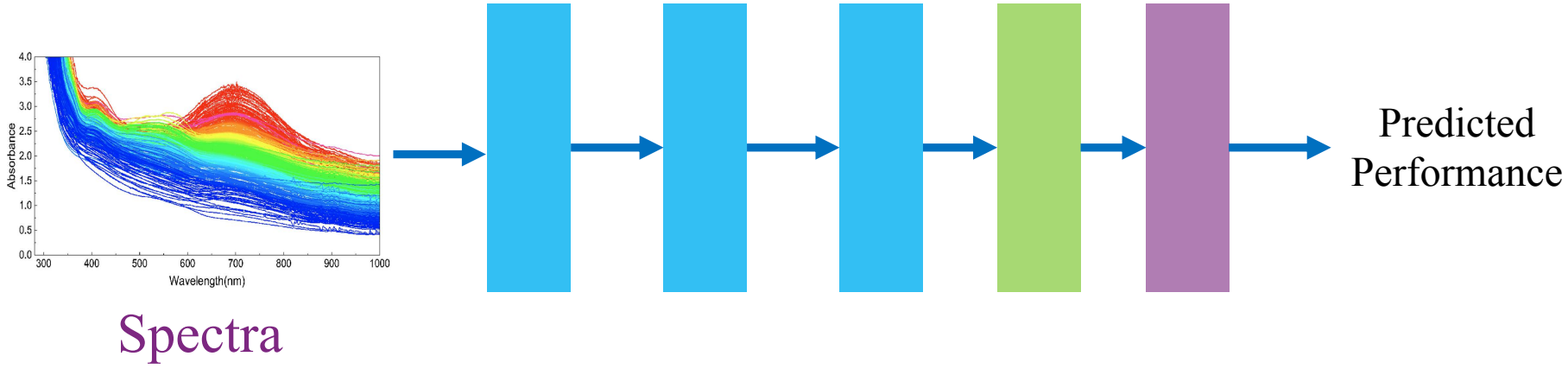

Flatten
FC
Absorbance
Wavelength(nm)
Spectra
Predicted
Composition

VAE(variational Autoencoder) Model



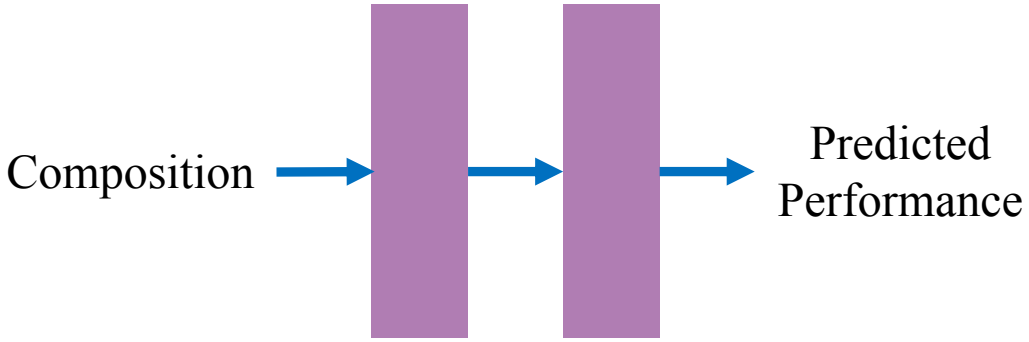
Variational Autoencoders | Generative AI Animated: www.youtube.com/watch?v=qJeaCHQ1k2w&t=96s

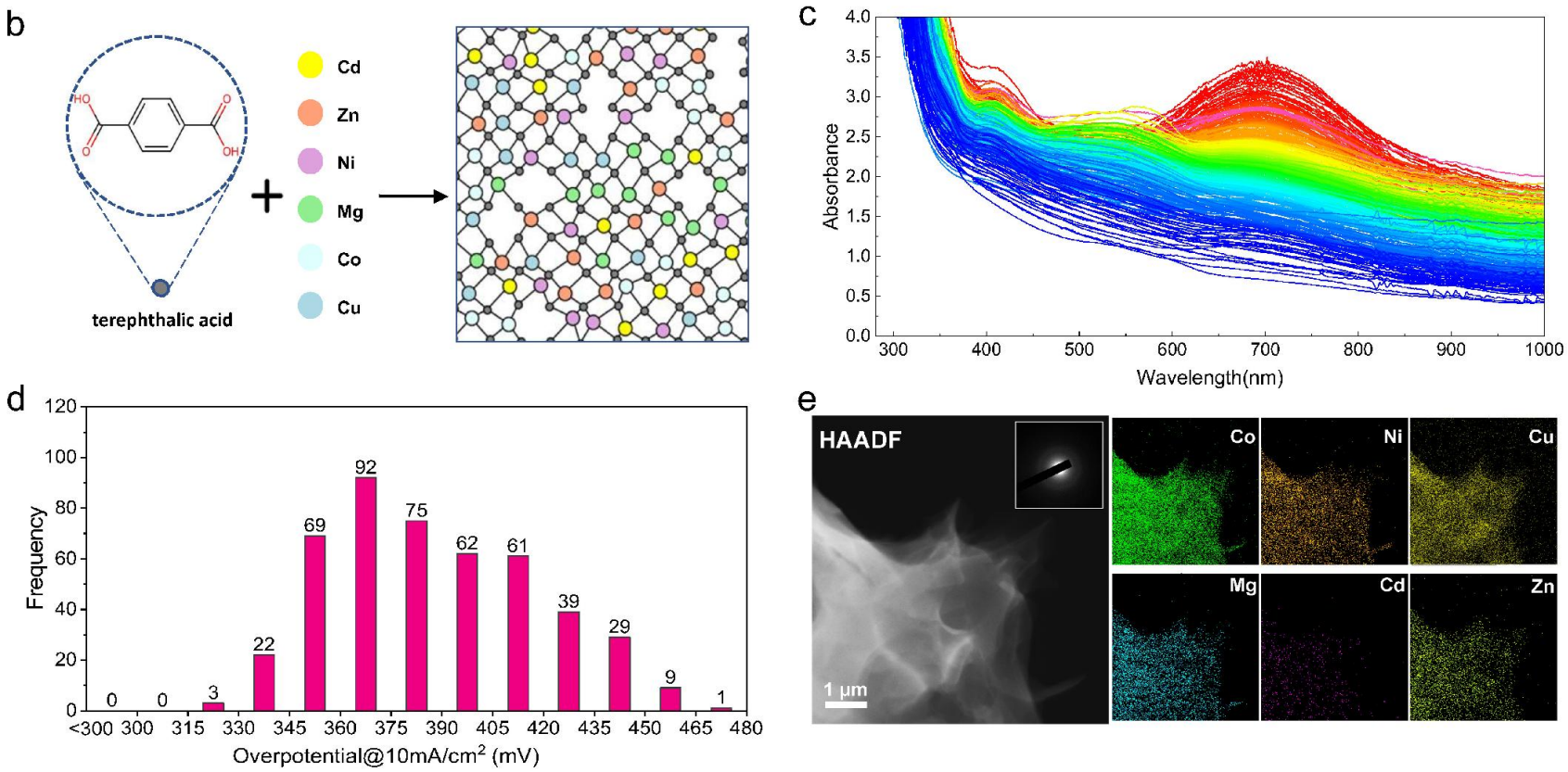
S2P Model



Spectra

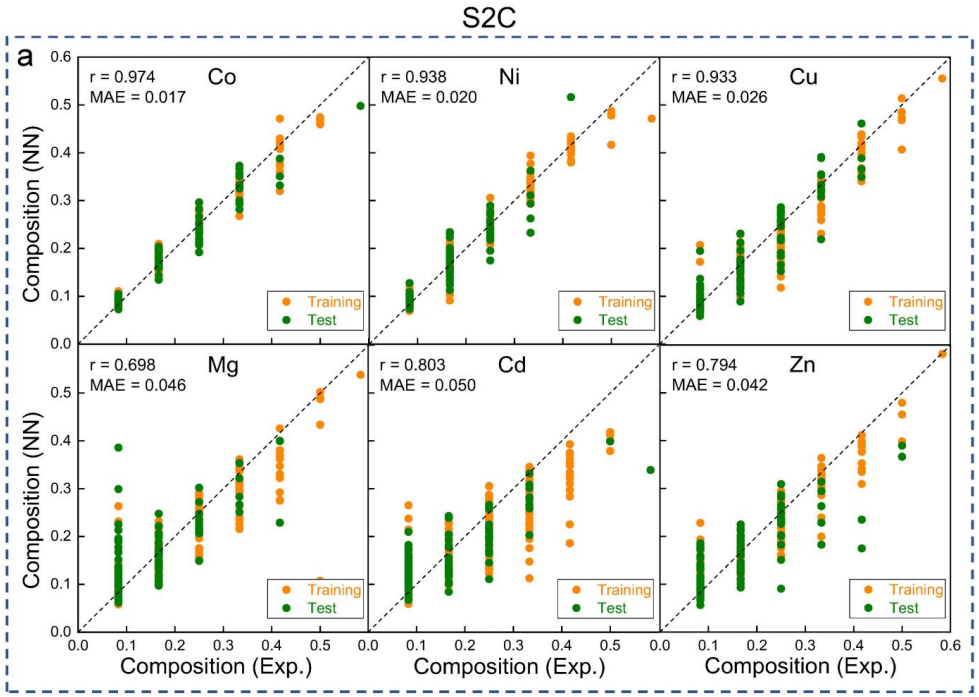
C2P Model

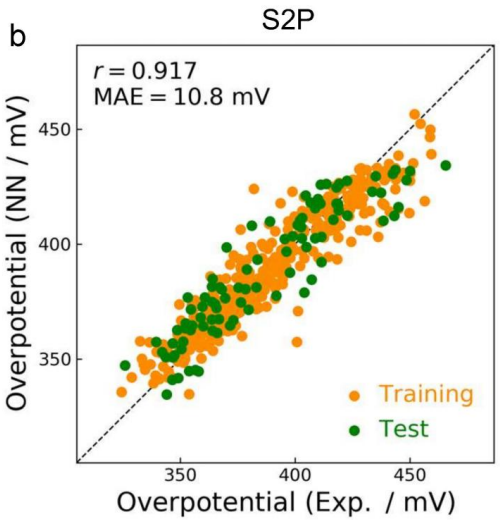




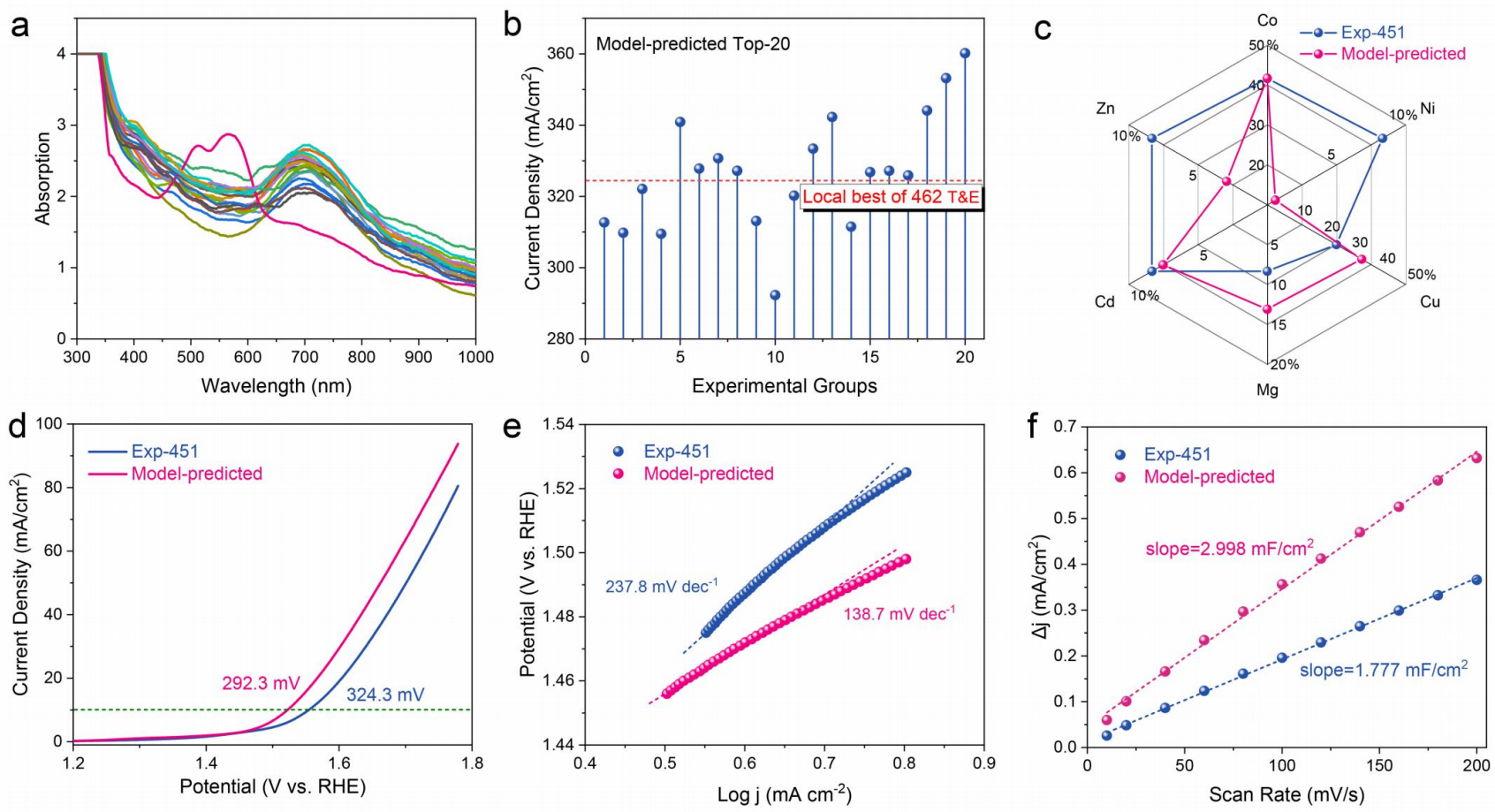
A diverse library of high-entropy catalysts was prepared by systematically varying the ratios of six divalent metals (Co, Ni, Cu, Mg, Cd, Zn) incorporated into a hybrid metal-organic structure with terephthalic acid

Using a high-throughput, automated wet-chemistry approach, 462 catalysts were synthesized and characterized

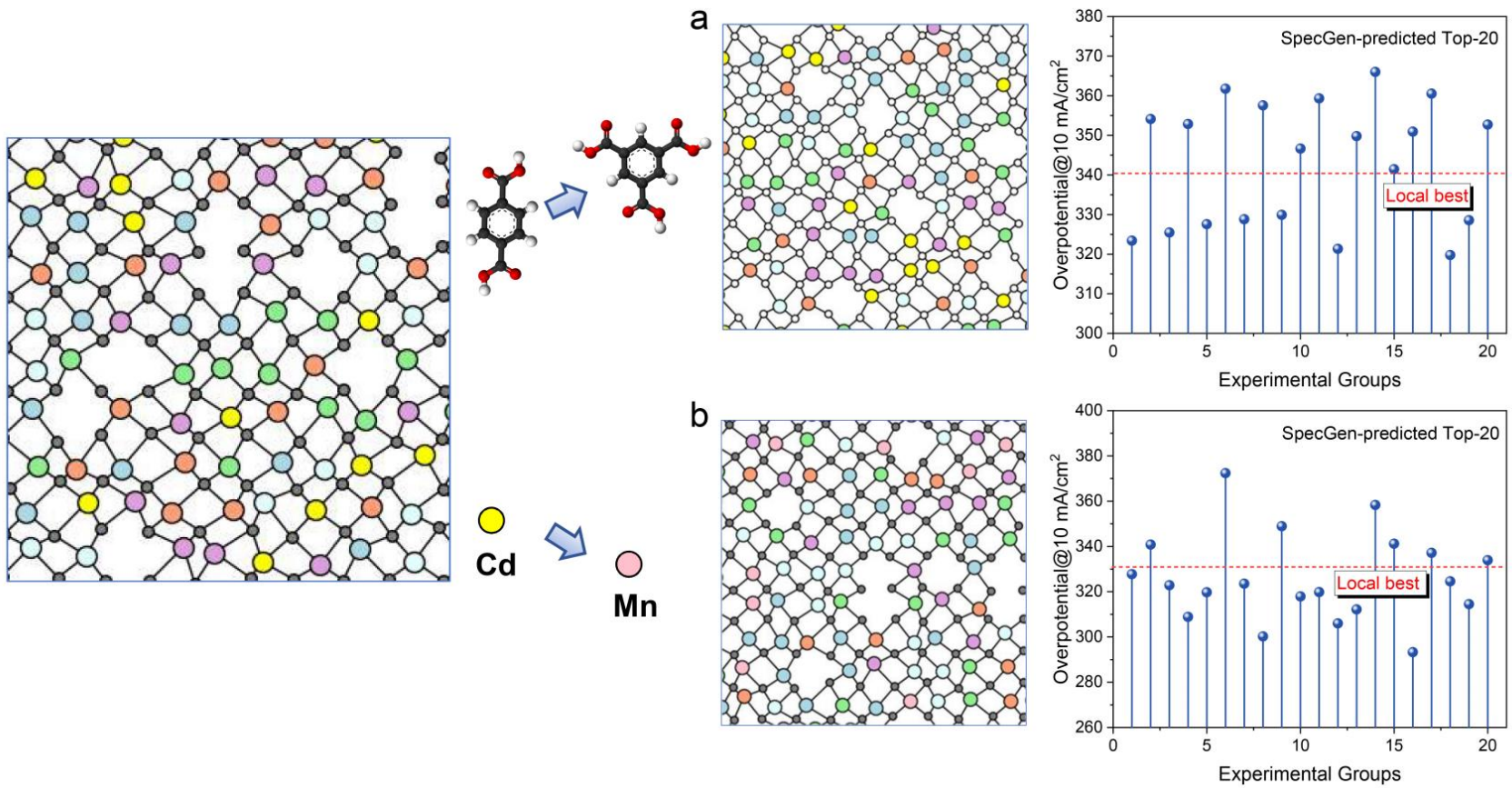




- It achieved a Spearman correlation of 0.996 between the experimental spectra and those reconstructed from the VAE latent space.
- The S2C module showed excellent predictive accuracy on an independent test set.
- S2P yielded a high correlation of 0.917 between predicted and experimental overpotentials. The mean absolute error (MAE) of these overpotential measurements was 10.8 mV.



Following a rapid screen for efficient senary high-entropy catalysts, the spectroscopic generative model further optimized the top-performing candidate, lowering its overpotential at 10 mA/cm^2 by an additional 32 mV.



SpecGen demonstrates strong transferability when chemical environment changes are moderate, but its generalization ability is limited when the system undergoes fundamental alterations in electronic structure.

Conclusion

- Spectroscopic descriptor-driven inverse design outperforms trial-and-error approaches

- Integration of AI and robotics enables autonomous catalyst discovery

Source Code: github.com/Tony935/SpecGen

Thank You