Alleviating the Energy Crisis: A Novel Multi-Task Machine Learning Algorithm for Designing Efficient Nanocatalysts to Reduce Industrial Energy Impact

THE ENERGY CRISIS

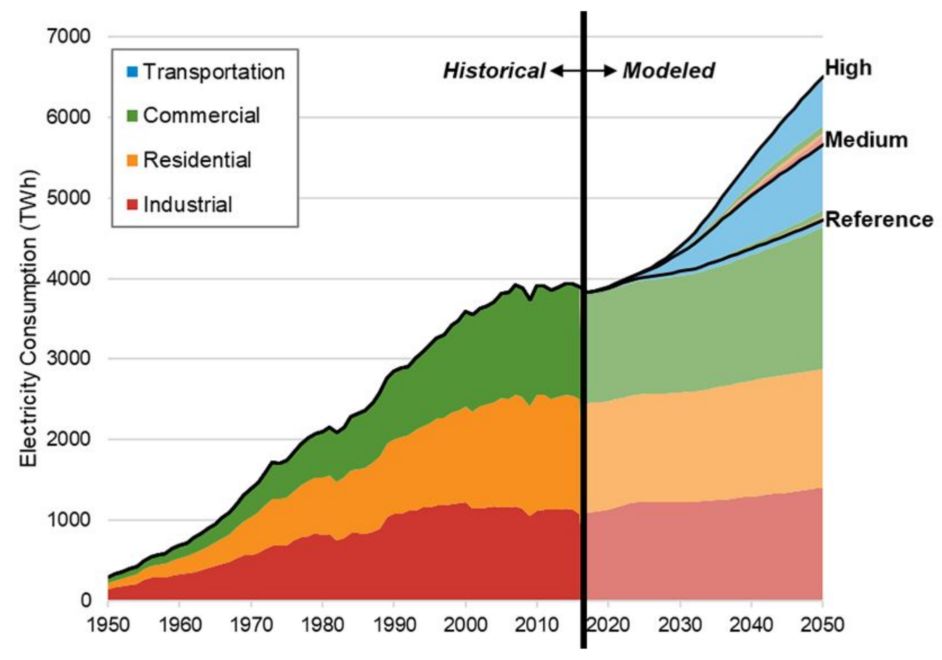

Fig 1. “Electrification Future Study: Scenarios of Electric Technology Adoption and Power Consumption in the United States.” Energy.gov.

There is a significant—and rising—gap between sources of energy and energy consumption, which has led in recent years to the largest energy crisis since the 1980s. Because it is hard to change household energy consumption, I targeted industrial use. This allows sustainable energy sources to catch up to demand and create a smoother transition away from fossil fuels.

Currently, many catalysts used in production are outdated and costly. I demonstrate a method which aids in the design of optimal catalysts. In addition, I illustrate high-speed analysis of catalysts for efficiency in design.

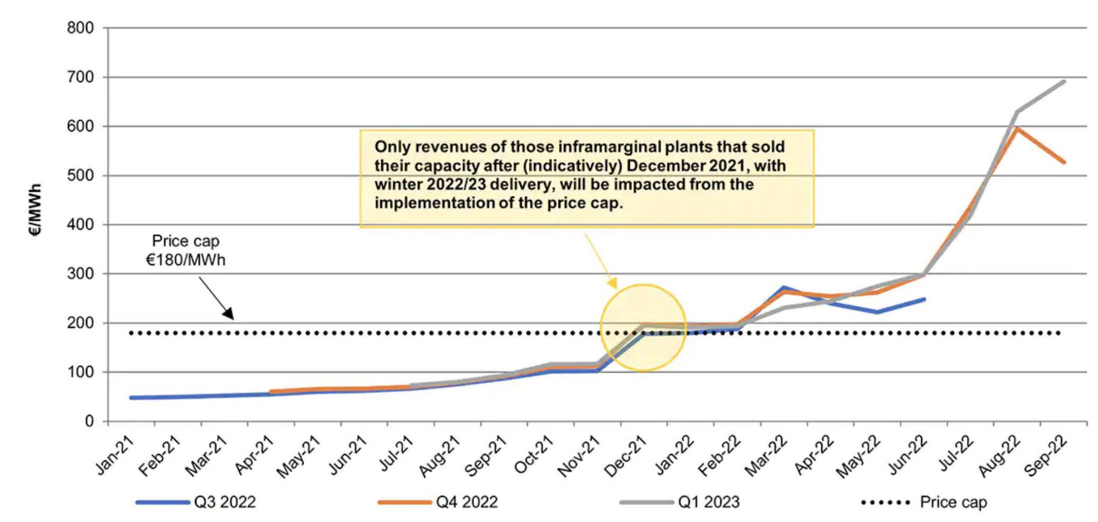

Fig 2. “Weekly Pricing Pulse: Commodities down as Energy Crisis Recedes.” IHS Markit, 23 Feb. 2023.

METHODOLOGY

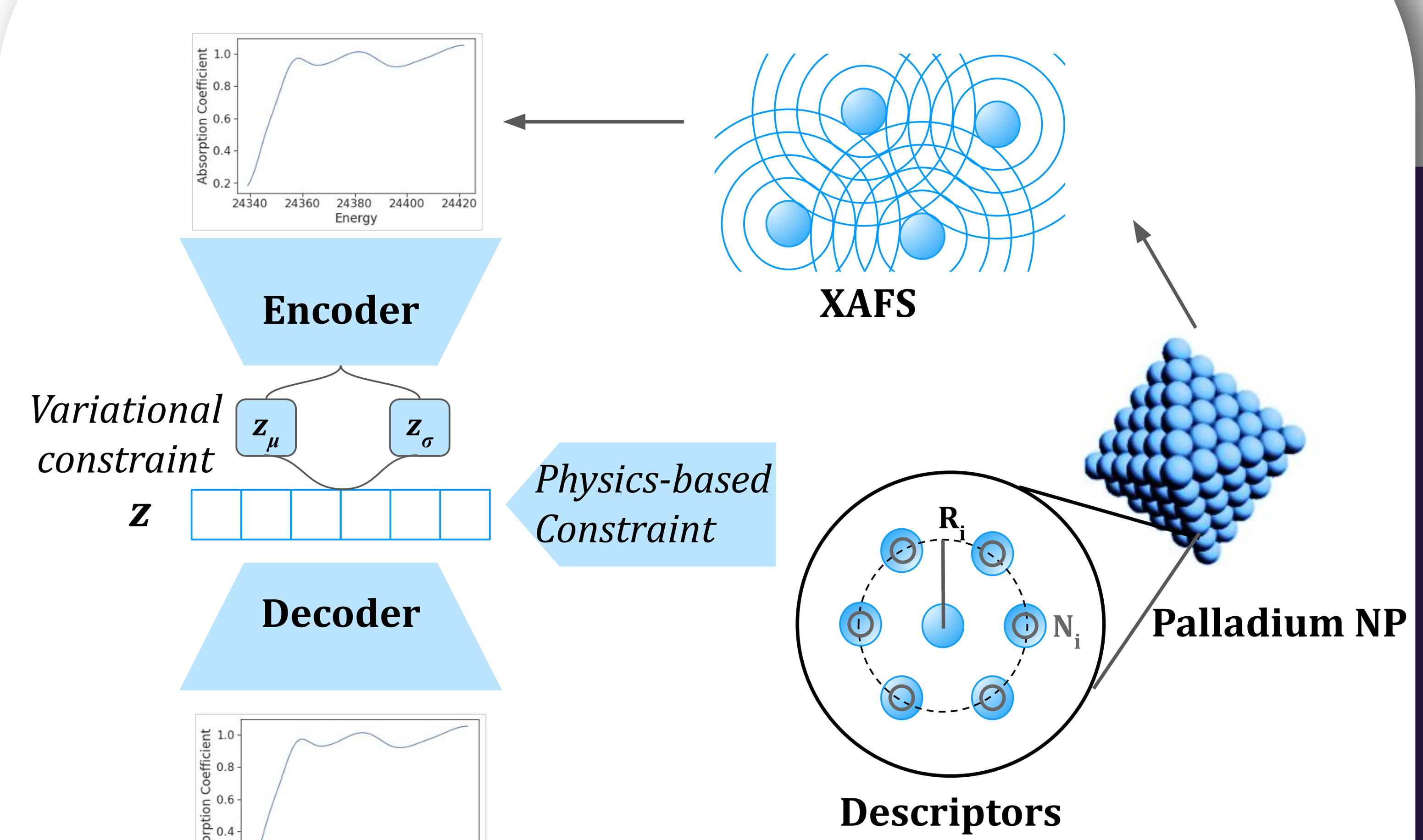

Fig 3. Overview of MAVEN methodology.

I designed a machine learning algorithm which satisfies two capabilities: to design new, optimized catalysts based on preselected characteristics; and, to perform real-time analysis of X-ray absorption spectroscopy that is hundreds of times faster than traditional methods. The **Multi-task Algorithm for Variational auto-ENcoding** (MAVEN) uses a novel mathematical framework that incorporates both **physics-informed and statistics-informed constraints**.

RESULTS

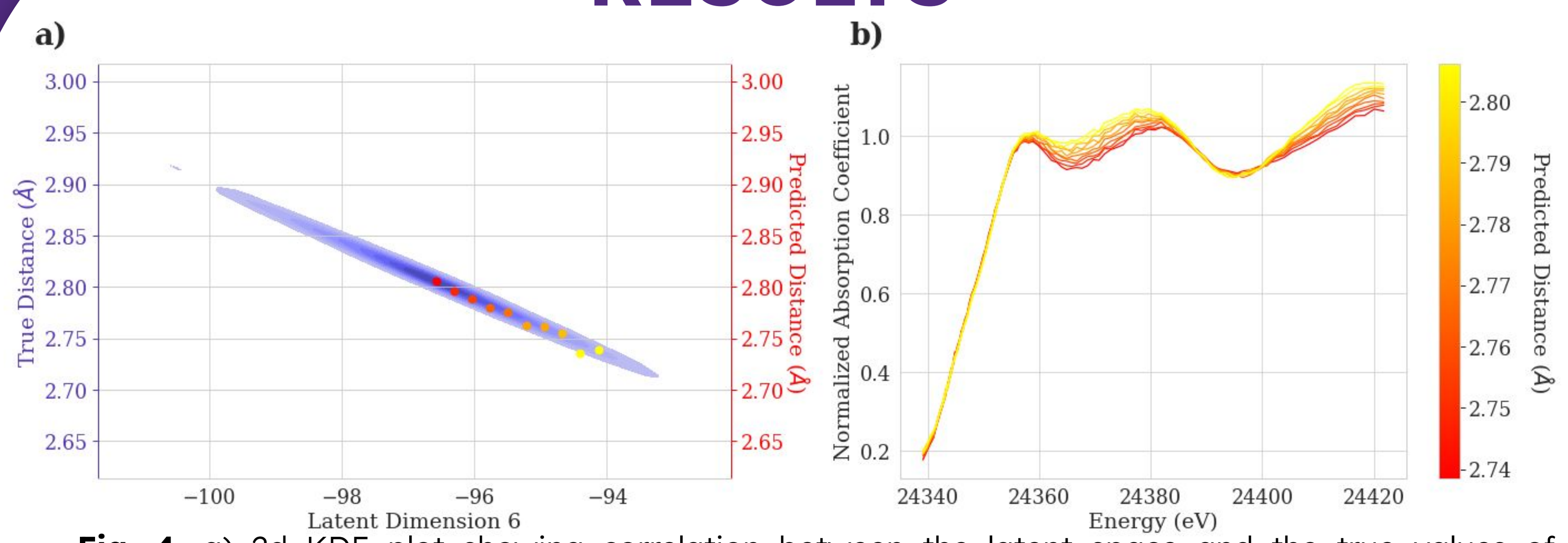

Fig. 4. a) 2d KDE plot showing correlation between the latent space and the true values of interatomic distance. Interpolation across latent space dimension 6 and their predicted values are overlaid. b) Generated XANES spectra from corresponding interpolated values shown in a).

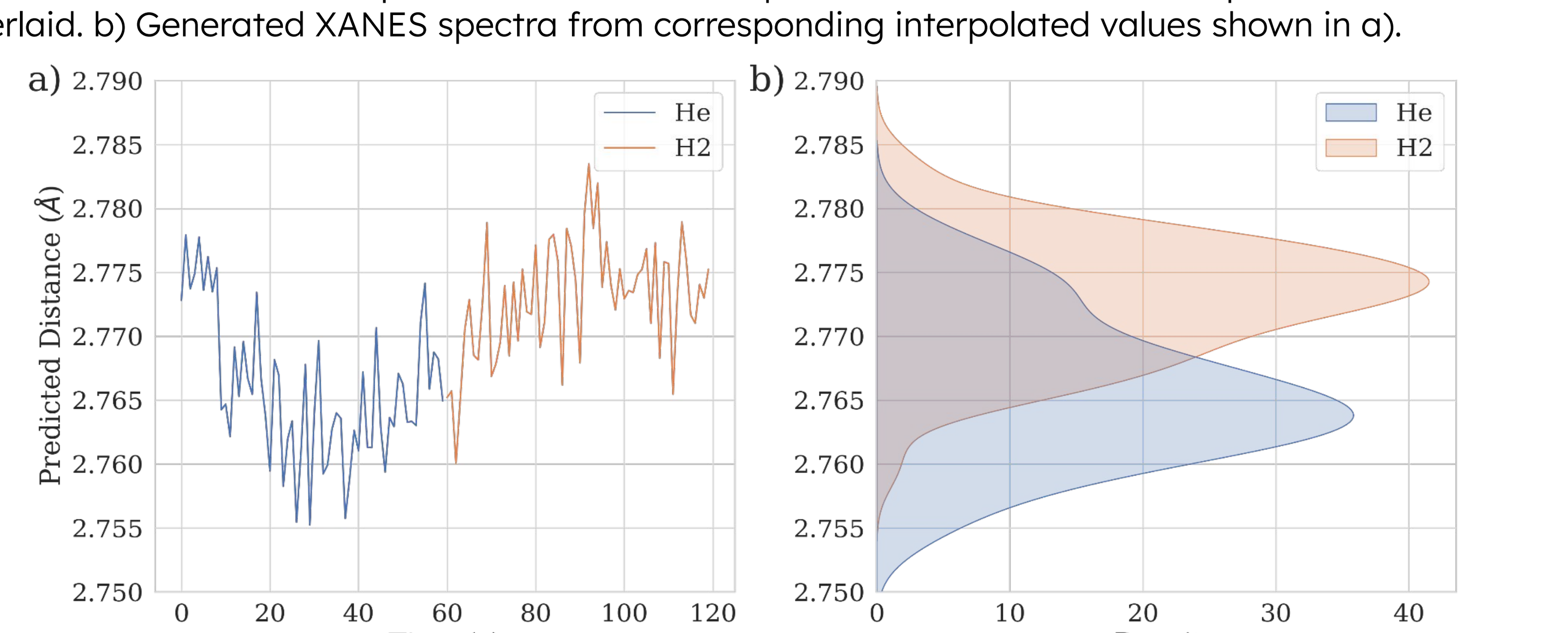

Fig. 5. a) The evolution of palladium hydride over time, where the atmosphere is helium in the first 60 seconds and is modulated to hydrogen in the last 60 seconds. b) A 1d KDE plot showing the distribution of predicted first shell interatomic distances between hydrogen and helium atmospheres.

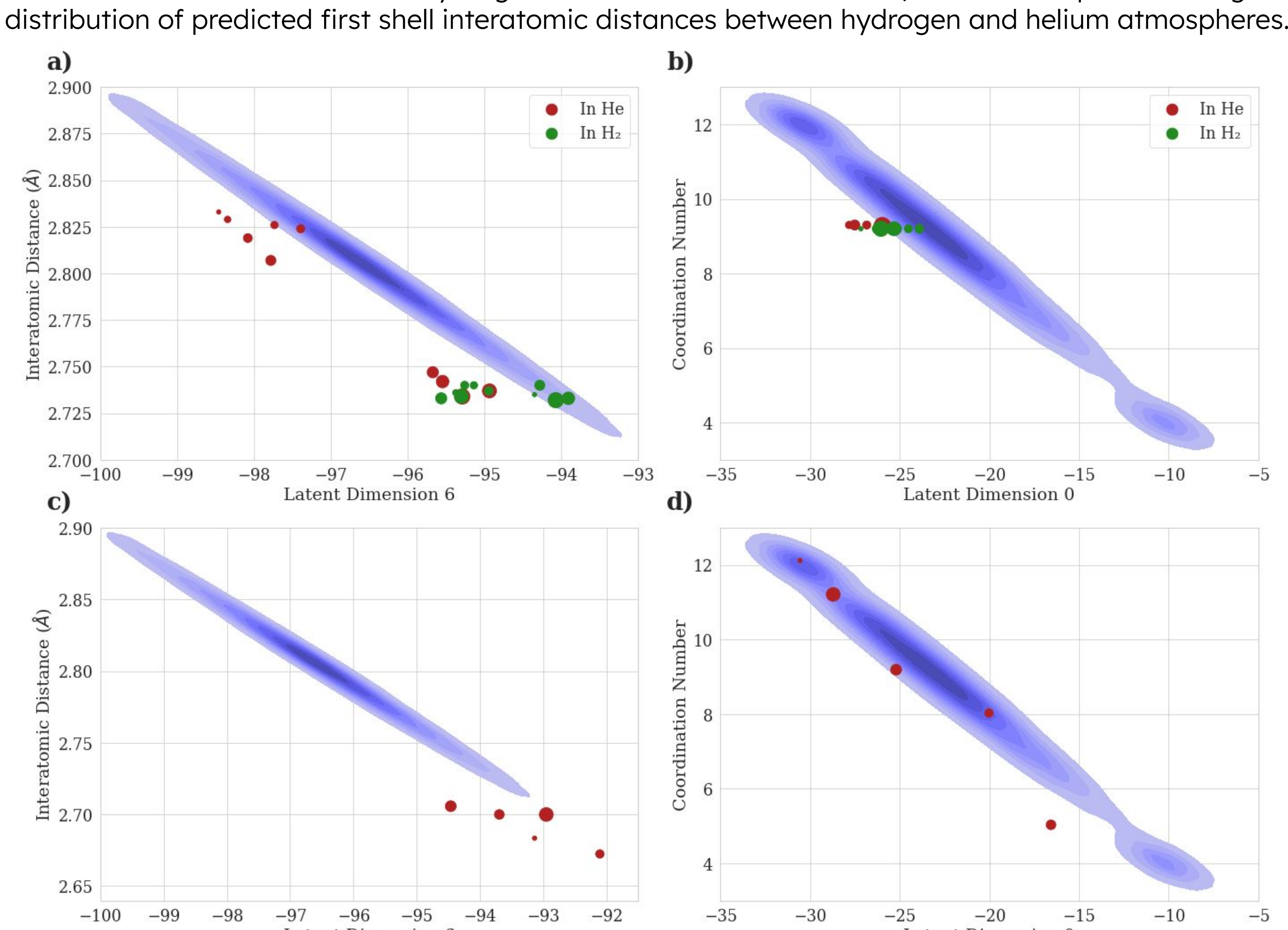

Fig. 6. A correlation plot between dimensions of the MAVEN latent space and the predicted descriptors sharing the highest mutual information with them. In purple is theoretical data not used in training, and in red and green are experimental data points in helium and hydrogen atmosphere, respectively. The temperature of each sample is denoted by the size of the point.

CONCLUSIONS

1. Explainability

MAVEN demonstrates interpretability because scientists can understand the relationships between spectra and properties using the latent space as a proxy (as seen in fig. 6). It is well established that a major problem with deep learning is explainability, or it is not possible to manage.

2. Interpolation for Materials Discovery

Interpolations along known nanocatalyst descriptors give insight when inverting the effects of properties on spectra and materials. While previous methodologies were able to decode structure from spectra and simulations were able to construct spectra from structural parameters, my algorithm is the first to be able to reverse-engineer materials in a self-consistent manner (as demonstrated in fig. 4). I can pinpoint the material at previously unknown points in the latent space with pre-selected nanocatalyst properties so that I can find optimized solutions for manufacturing.

3. Real-time identification of nanocatalyst properties

I demonstrate that MAVEN provides faster and more accurate identification of crucial properties for designing optimal nanocatalysts than state-of-the-art techniques for materials analysis. In previous methodologies, there was an unsatisfactory degree of accuracy in experimental data due to a lack of denoising capability, which would inhibit this from being used in real-world industrial situations. MAVEN allows for the understanding of physicochemical properties in complex, fast reactions through incomplete, noisy, time-modulated data, demonstrated in fig. 5 and fig. 6.

REFERENCES

1. IEA. “Renewable Electricity Growth Is Accelerating Faster than Ever Worldwide, Supporting the Emergence of the New Global Energy Economy - News.” IEA, 2021, www.iea.org/news/renewable-electricity-growth-is-accelerating-faster-than-ever-worldwide-supporting-the-emergence-of-the-new-global-energy-economy.
2. Molnar, Gergely, and Peter Levi. “How the Energy Crisis Is Exacerbating the Food Crisis – Analysis.” IEA, 14 June 2022, www.iea.org/commentaries/how-the-energy-crisis-is-exacerbating-the-food-crisis.
3. Liang, Zhu, et al. “Decoding Structure-Spectrum Relationships with Physically Organized Latent Spaces.” Physical Review Materials, vol. 7, no. 5, 16 May 2023, https://doi.org/10.1103/physrevmaterials.7.053802. Accessed 20 Nov. 2023.
4. Linardatos, Pantelis, et al. “Explainable AI: A Review of Machine Learning Interpretability Methods.” Entropy, vol. 23, no. 1, 25 Dec. 2020, p. 18, www.mdpi.com/1099-4300/23/1/18, https://doi.org/10.3390/e23010018.