

Are dielectrics a viable alternative to commercial energy storage?

Dielectrics are essential for modern energy storage, but currently have limitations in energy density and thermal stability. Here, the authors discover dielectrics with 11 times the energy density of commercial alternatives at elevated temperatures.

Why is a high thermal stability dielectric important?

For example, the high thermal stability of each dielectric in Fig. 3 b eliminates the need for capacitor cooling systems. Among these dielectrics, those with higher U_e are preferred, as this attribute reduces the amount of capacitor material required to store a fixed amount of energy.

Can artificial intelligence help converge on high-performance dielectrics?

Within the vast expanse of chemical possibilities for all polymers, it is likely that a wide variety of high-performance dielectrics await discovery. Well-trained and calibrated artificial intelligence (AI), capable of handling large numbers that challenge human imagination, can help converge on extraordinary materials rapidly.

How can a new generation of AI improve materials discovery?

Any of these approaches to materials discovery would benefit from increased accuracy of the polyGNN models--perhaps using strategies like pretraining 51, 52 --to reduce the amount of time spent on bad leads. Moreover, significant resources should be dedicated to a new generation of AI characterized by human interpretability.

Can machine learning be used to design polymers for energy storage capacitors?

Kern, J., Chen, L., Kim, C. & Ramprasad, R. Design of polymers for energy storage capacitors using machine learning and evolutionary algorithms. *J. Mater. Sci.* 56, 19623-19635 (2021). Gurnani, R. et al. polyG2G: a novel machine learning algorithm applied to the generative design of polymer dielectrics.

Does polyverse work in high-temperature dielectric search?

AI-ASSISTED DISCOVERY OF HIGH-TEMPERATURE DIELECTRICS FOR ENERGY STORAGE



This study introduces the polyVERSE ("polymers designed by Virtually-Executed Rule-Based Synthesis Experiments") paradigm (Fig. 1 a), showcasing its success in achieving these four attributes in the context of high-temperature dielectric search.



It is illustrated here how one may harness a rational co-design approach-involving synergies between high-throughput computational screening and experimental synthesis and testing-with the example of polymer dielectrics design for electrostatic energy storage applications. Although traditional materials discovery has historically benefited from ???



High-temperature dielectric polymers are in high demand for powering applications in extreme environments. Here, we have developed high-temperature homopolymer dielectrics with anisotropy by leveraging the hierarchical structure in semicrystalline polymers. The lamellae have been aligned parallel to the surface in the dielectric films.

AI-ASSISTED DISCOVERY OF HIGH-TEMPERATURE DIELECTRICS FOR ENERGY STORAGE



AI-assisted discovery of high-temperature dielectrics for energy storage, 2024 7 19
Nature Communications .

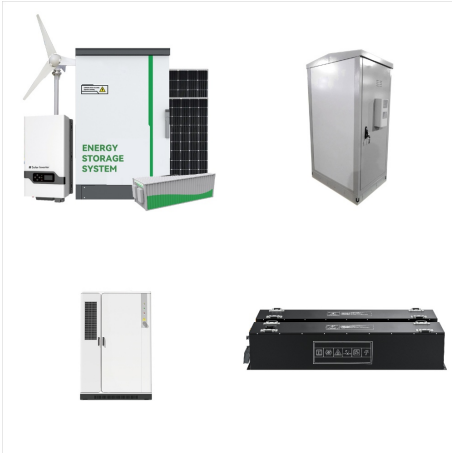


Dielectrics are essential for modern energy storage, but currently have limitations in energy density and thermal stability. Here, the authors discover dielectrics with 11 times the energy



Rishi Gurnani & Stuti Shukla & Deepak Kamal & Chao Wu & Jing Hao & Christopher Kuenneth & Prithish Aklujkar & Ashish Khomane & Robert Daniels & Ajinkya A. Deshmukh & Yang Cao & Gregory Sotzing & Rampi, 2024. "AI-assisted discovery of high-temperature dielectrics for energy storage," Nature Communications, Nature, vol. 15(1), pages 1-10, December.

AI-ASSISTED DISCOVERY OF HIGH-TEMPERATURE DIELECTRICS FOR ENERGY STORAGE



Electrostatic capacitors are critical components in a broad range of applications, including energy storage and conversion, signal filtering, and power electronics [1], [2], [3], [4]. Polymer-based materials are widely used as dielectrics in electrostatic capacitors due to their high voltage resistance, flexibility and cost-effectiveness [5], [6], [7].



Polymer dielectrics are promising for high-density energy storage but dielectric breakdown is poorly understood. AI-assisted discovery of high-temperature dielectrics for energy storage



AI-assisted discovery of high-temperature dielectrics for energy storage polymer dielectrics for high-temperature capacitors need to meet multiple property criteria, including a high energy density to reduce the size of capacitors, high thermal stability to survive high operating temperatures, and high breakdown field strength to withstand

AI-ASSISTED DISCOVERY OF HIGH-TEMPERATURE DIELECTRICS FOR ENERGY STORAGE



[3] Yifei Wang, Zongze Li, Chao Wu, Peinan Zhou, Jierui Zhou, Jindong Huo, Kerry Davis, Antigoni Konstantinou, Hiep Nguyen, and Yang Cao, "High-performance polymer dielectric with montmorillonite nanosheets coating for high-temperature energy storage ", Chemical Engineering Journal, Vol. 437, 135430, 2022.



Many of the discovered dielectrics exhibit high thermal stability and high energy density over a broad temperature range. One such dielectric displays an energy density of 8.3 J cc⁻¹ at

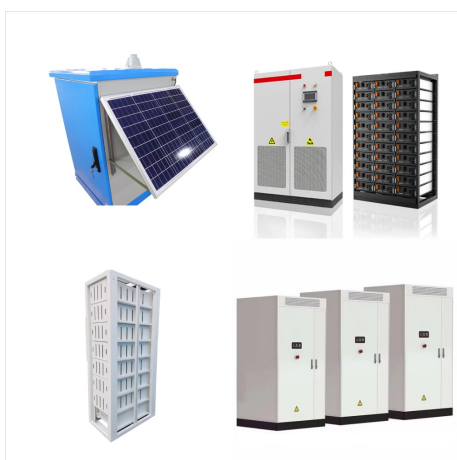


Many of the discovered dielectrics exhibit high thermal stability and high energy density over a broad temperature range. One such dielectric displays an energy density of 8.3 J cc⁻¹ at 200 °C, a value 11 x that of any commercially available polymer dielectric at this temperature.

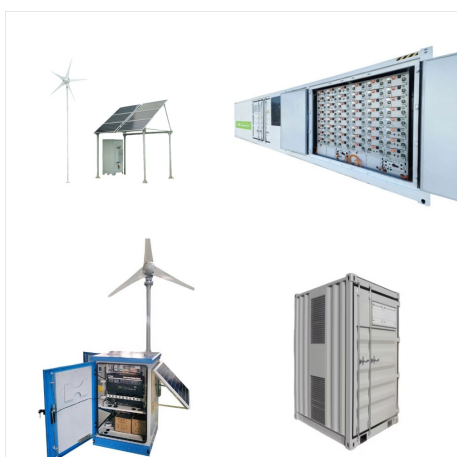
AI-ASSISTED DISCOVERY OF HIGH-TEMPERATURE DIELECTRICS FOR ENERGY STORAGE



This work was financially supported by the Office of Naval Research through a Multi-University Research Initiative (MURI) grant (N00014-17-1-2656), the Center for Understanding and ???



"The new class of polymers with high energy density and high thermal The potential for real-world translation of AI-assisted materials AI-assisted discovery of high-temperature dielectrics



AI-assisted discovery of high-temperature dielectrics for energy storage Article Open access 19 July 2024 Designing polymer nanocomposites with high energy density using machine learning

AI-ASSISTED DISCOVERY OF HIGH-TEMPERATURE DIELECTRICS FOR ENERGY STORAGE



Here, P_{max} and P_r represent the maximum polarization and remanent polarization, and η denotes the energy efficiency. These equations demonstrate that high P_{max} , low P_r and high dielectric breakdown field E_b are conducive to achieving higher energy density and energy efficiency in dielectric materials. Owing to the rich characteristics of multiscale ???



Polymer dielectrics are considered promising candidate as energy storage media in electrostatic capacitors, which play critical roles in power electrical systems involving elevated temperatures



???AI-assisted discovery of high-temperature dielectrics for energy storage???, 2024 7 19
???Nature Communications??????? . ???

AI-ASSISTED DISCOVERY OF HIGH-TEMPERATURE DIELECTRICS FOR ENERGY STORAGE



AI-assisted discovery of high-temperature dielectrics for energy storage. Overview of attention for article published in Nature Communications, July 2024. AI-assisted discovery of high-temperature dielectrics for energy storage Published in: Nature Communications, July 2024 DOI: 10.1038/s41467-024-50413-x:



AI-assisted discovery of high-temperature dielectrics for energy storage - Nature Communications This multi-disciplinary AI-assisted design and validation journey has led to a remarkable class



Polymer dielectrics are key components for electrostatic capacitors in energy, transportation, military, and aerospace fields, where their operation temperature can be boosted beyond 125 °C. While most polymers bear poor thermal stability and severe dielectric loss at elevated temperatures, numerous linear polymers with linear D-E loops and low dielectric ???

AI-ASSISTED DISCOVERY OF HIGH-TEMPERATURE DIELECTRICS FOR ENERGY STORAGE



Machine learning has shown its great potential in the accelerated discovery of advanced materials in the field of computational molecular design. High-temperature polymer dielectrics are urgently required with the emerging applications of energy-storage dielectric film capacitors under high-temperature conditions. Here, we demonstrate the successful prediction ???