Unveiling the key factors that determine properties of porous polymer materials

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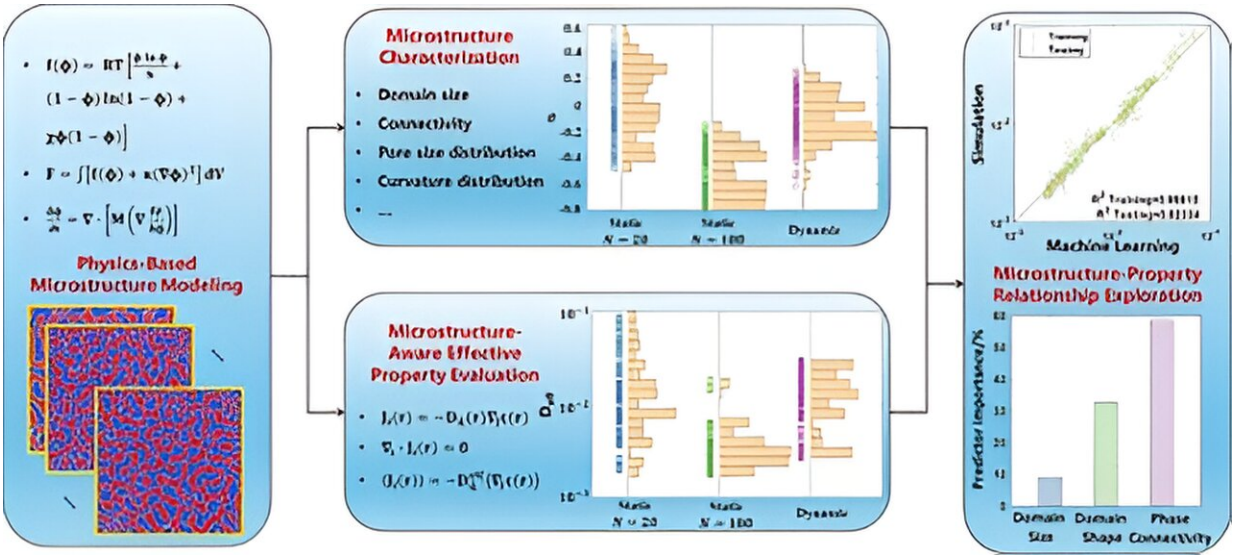

Credit: *ACS Applied Materials & Interfaces* (2024). DOI: 10.1021/acsami.4c03011

Determining the relationship between microstructure features and their properties is crucial for improving material performance and advancing the design of next-generation structural and functional materials. However, this task is inherently challenging.

To address the challenges, LLNL scientists have developed an efficient and comprehensive computational framework to decipher implications

of porous microstructures and their properties. The research appears in the journal *ACS Applied Materials & Interfaces*.

"We have developed an integrated computational framework which incorporates physics-based microstructure modeling, microstructure feature extraction, microstructure-aware effective property evaluation and machine-learning analysis tools," said Longsheng Feng, LLNL scientist and lead author of the paper.

The team applied the framework to polymer-based porous materials as a representative model system and demonstrated its capability to explore how polymerization dynamics influence various general and local microstructure features like domain size and pore size distribution, and how these features impact transport properties.

"Our objective is to establish a framework capable of understanding not only the formation of microstructures using physics-based models and evaluating their effective properties, but also aims to discern which microstructure features dictate different properties and how they do so," said Tae Wook Heo, LLNL scientist and co-author of the paper.

This approach offers a novel framework for assessing microstructure–property relationships in polymer-based porous materials, paving a way for the development of advanced materials.

"Understanding these relationships can guide the processing procedures to tailor specific microstructures to achieve desired properties of polymeric porous materials for various applications, such as membranes," said Juergen Biener, LLNL scientist and co-author of the paper.

LLNL scientist Sijia Huang also contributed to this paper.

More information: Longsheng Feng et al, Integrated Framework to Model Microstructure Evolution and Decipher the Microstructure–Property Relationship in Polymeric Porous Materials, *ACS Applied Materials & Interfaces* (2024). DOI: 10.1021/acsami.4c03011

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