

Abstract Submitted  
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**Nanostructure and free volume effects in enhancing the dielectric response of strongly dipolar polymers** RUI DONG, North Carolina State Univ, YASH THAKUR, Penn State Univ, VIVEK RANJAN, North Carolina State Univ, MARCO BUONGIORNO NARDELLI, North Texas Univ, QIMING ZHANG, Penn State Univ, JERRY BERNHOLC, North Carolina State Univ — Materials for capacitive energy storage with high energy density and low loss are desired in many fields. We perform multiscale simulations to investigate several members of the aromatic polyurea family. We find that the disordered structures with misaligned chains have considerably larger dielectric constants, due to significant increase in the free volume, which leads to easier reorientation of dipolar groups in the presence of an electric field. Large segment motion is still not allowed below the glass transition temperature, upholding the very low loss at high field and elevated temperature that we observe experimentally. Optimization of the nanostructure and free volume effects thus provides a new, very promising pathway for the design of high-performance dielectrics for capacitive energy storage.

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