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Multiscale simulations of polyurea-based dielectrics for capacitive energy storage RUI DONG, VIVEK RANJAN, North Carolina State Univ, MARCO BUONGIORNO NARDELLI, University of North Texas, JERZY BERNHOLC, North Carolina State Univ — In high energy capacitors, bi-axially oriented polypropylene is the preferred the state-of-art low loss dielectric. However, its energy density only reaches 4 J/cm^3 at 600 MV/m with 85% efficiency, while the recently synthesized polythiourea reaches 8 J/cm^3 with 95% efficiency under the same conditions [1]. Members of the aromatic polyurea family [2] have also been reported to have similarly high energy densities. We have performed multiscale simulations to investigate several members of the polyurea/ polythiourea family, focusing on their structural and dielectric properties. Antiparallel packing of urea/thiourea units is found to be preferred energetically, but the energy surfaces are remarkably flat overall, with several distorted and disordered structures being energetically close. Nevertheless, microscopic geometries are found to be critical for the ionic response. Local disorder leads to larger permittivities, but also increased losses. [1] Wu et al, Advanced Material, 25, 1734 (2013). [2] Wang et al, APL 94, 202905 (2009).

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