Abstract Submitted
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Modelling and multiscale simulations of meta aromatic polyurea: microscopic geometry and dielectric properties RUI DONG, VIVEK RANJAN, North Carolina State Univ, MARCO BUONGIORNO NARDELLI, University of North Texas, JERZY BERNHOLC, North Carolina State Univ — BOPP is the state-of-art material for high-power-density capacitors. However, its efficiency drastically drops at high electric fields. Recently, polymers in the polyurea/polythiourea family have been shown to have much higher energy density and efficiency at high fields than BOPP [1-2]. We perform multiscale simulations to investigate dielectric and structural properties of meta aromatic polyurea (mAP). Both crystalline and disordered structures have been studied, and much larger ionic contribution to permittivity is found in disordered structures. The specific volume is 10% to 20% larger in the latter, leading to greater structural flexibility. For example, the orientation variations of polar units are 100% larger than in the crystal structure, and the phonon density of states in the low frequency regime is significantly enhanced. At the same time, we find that meta aromatic polyurea has a higher tendency to be disordered than other members in the polyurea family. All these facts lead to a significantly larger permittivity of mAP.

[1] Wu et al, Advanced Materials, 25, 1734 (2013).
[2] Wang et al, APL 94, 202905 (2009).

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