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MOF-Polymer Composites for Dielectrics

LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Early Career R&D Program

Sandia National Laboratories
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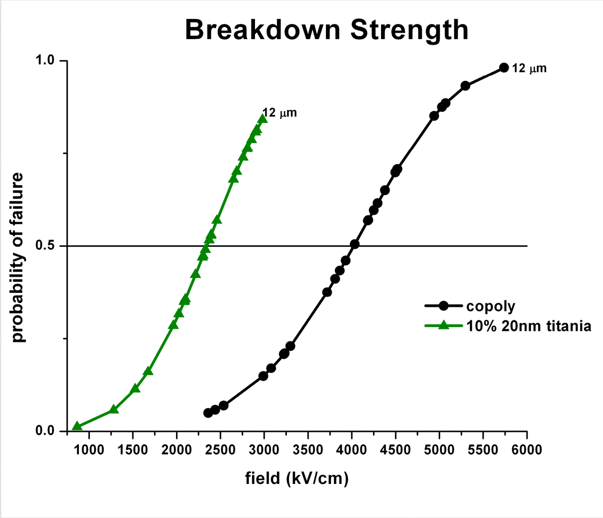
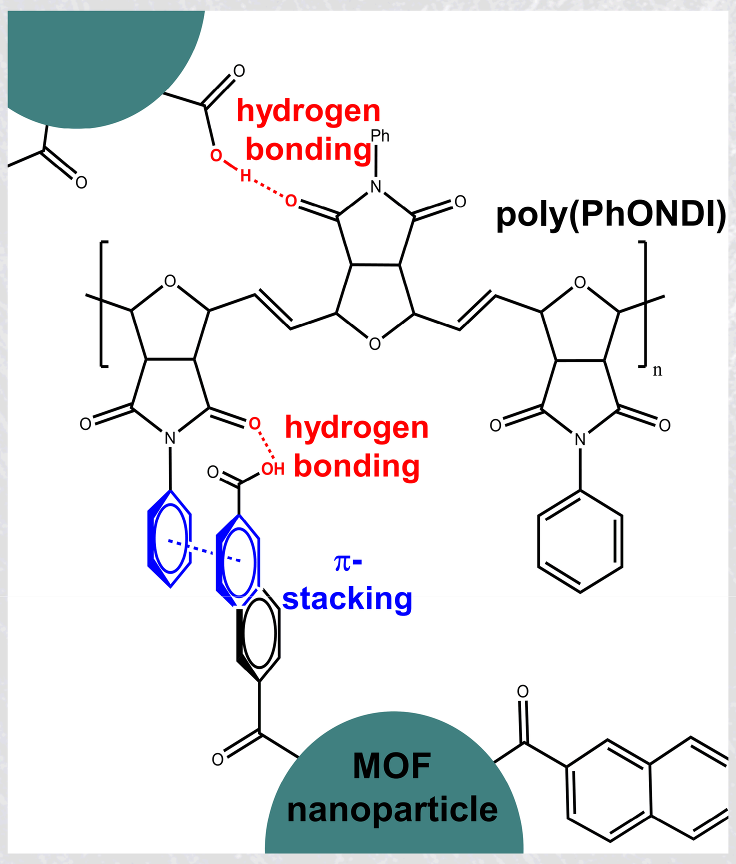
Problem

High performance capacitors require dielectric materials with high energy density, good temperature stability and soft failure modes. Polymer dielectrics offer many advantages , including high breakdown strengths and soft failure modes, but generally suffer from low energy densities, due to low permittivity values.



One technique to improve permittivity values is the use of inorganic/polymer composites. However, in many composites the benefits of increased permittivity are negated by a concomitant decrease in dielectric breakdown strength, resulting in no net improvement in energy density.

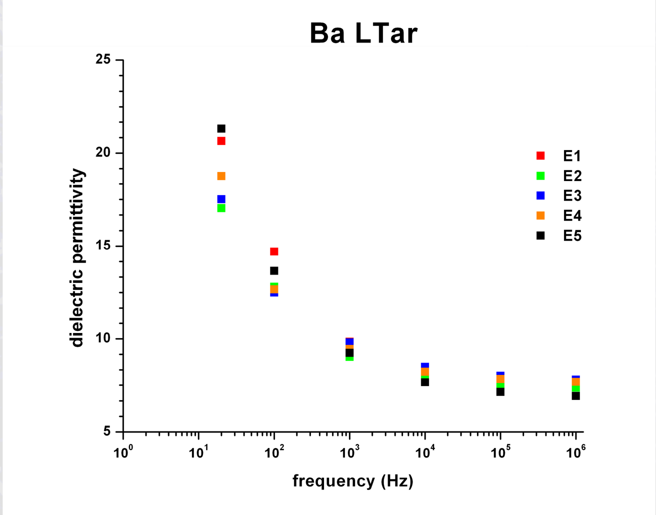
Approach



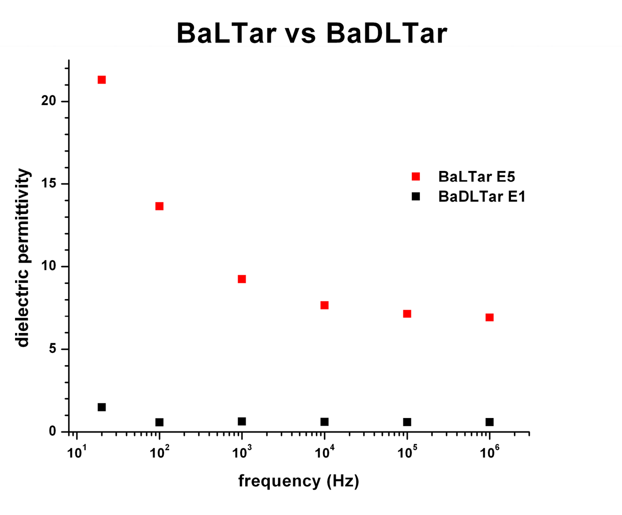
The poor breakdown performance of composites is often attributed to poor compatibility between the polymer and the inorganic filler, leading to poor dispersion and integration. We propose that metal-organic frameworks, which have intrinsic organic functionality, used as the filler in a MOF/polymer composite, may provide improved compatibility and dispersion, and yield composites with improved properties relative to traditional inorganic/polymer composites.

Results: MOF dielectric properties

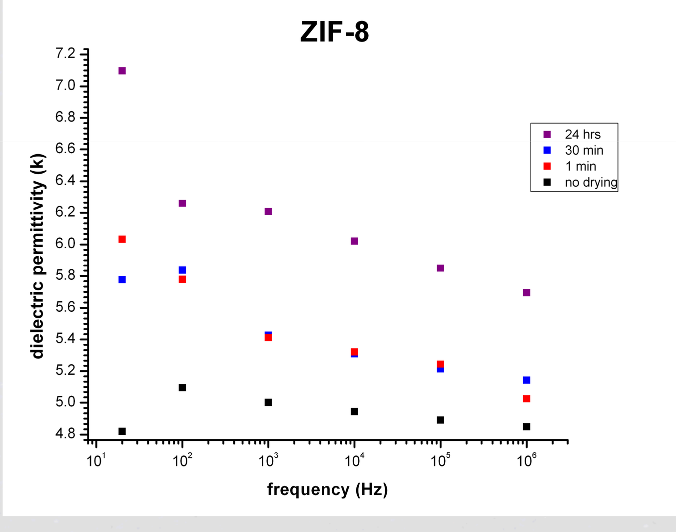
BaTar: microstructure, noncentro vs centro, effect on κ



BaLTar has much higher permittivity than BaDLTar



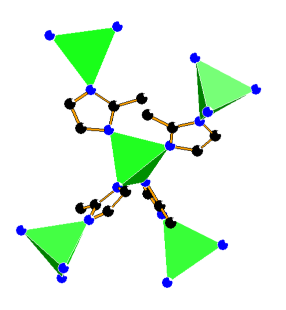
ZIF-8: measured permittivity much higher than theory (1.98)



- pressure induced amorphization
- solvent/water in pores
- density/microstructure

Drying/exposure to atmosphere induces large changes in κ, probably due to presence of small molecules in pores.

Results: Composites

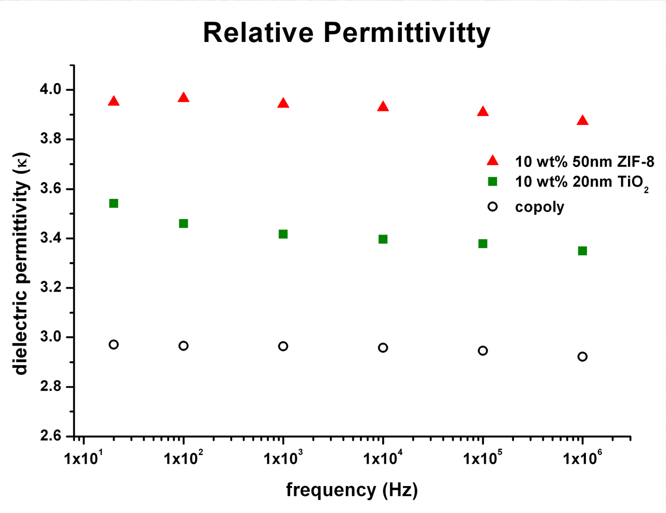


ZIF-8: [Zn(2-methylimidazolate)$_2$.2S]$_\infty$

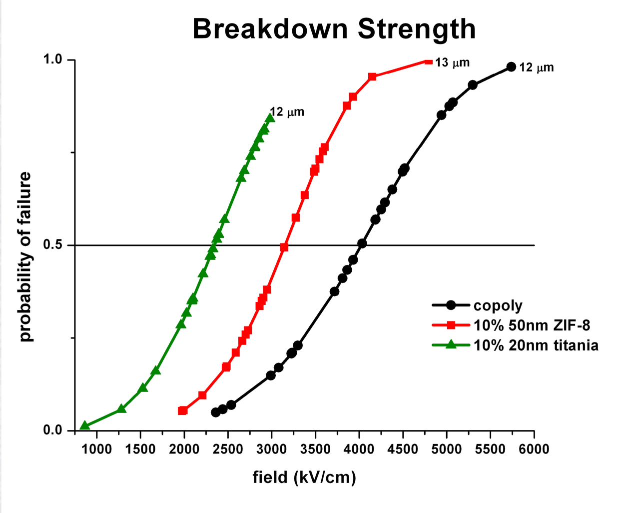
I -4 3 m cubic (sodalite)

ZIF-8 is a porous zeolitic imidazolate framework that can be readily synthesized in a variety of particle sizes.

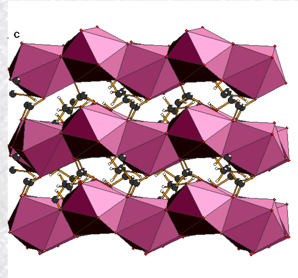
10 wt% ZIF-8/polymer composites of ~60nm particles have better dielectric permittivity and breakdown strengths than composites of 10wt% TiO_2/polymer.



ZIF-8 composite outperforms TiO_2 composite



Although the ZIF-8 composite outperforms the TiO_2 composite, due to the lower breakdown strength relative to the polymer alone, the energy density of the composite does not improve relative to the polymer.

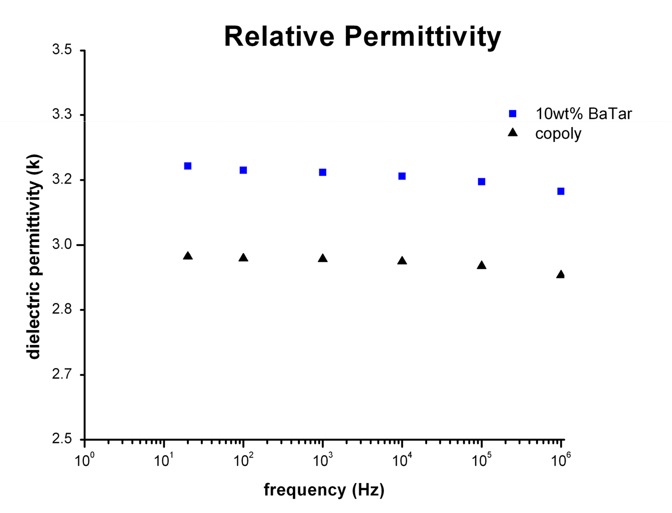


BaLTar: [Ba(L-tartrate)]$_\infty$

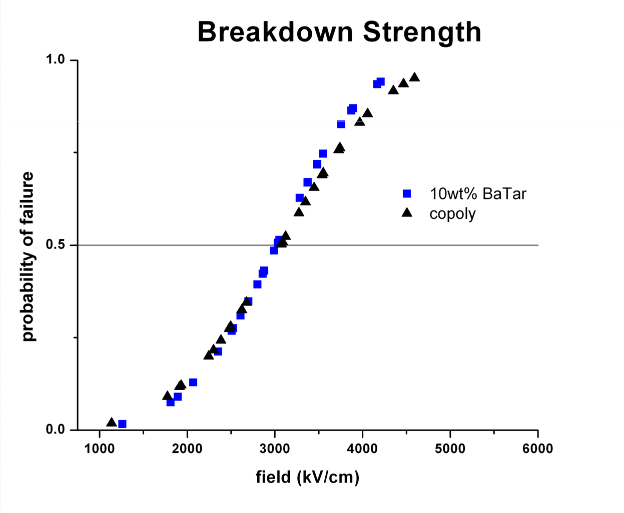
P 2_1 2_1 2_1 noncentrosymmetric

Ba(L-Tar) is a dense chiral framework stable to 250 °C.

10 wt% BaLTar/polymer composites of ~3-5um particles have breakdown strengths as high as those of the copolymer alone.



BaLTar composite maintains high breakdown strength



High breakdown strength is maintained, however, the small change in permittivity results in minimal improvements in energy density.

Significance/Future Work

Initial results on MOF/polymer composites are promising but further study is needed addressing:

- dispersion and reproducibility
- particle size effects
- particle surface functionalization
- additional polymer types
- particle/polymer functionality interplay
- covalent integration
- dielectric properties of pure MOFs

MOFs provide an alternative to traditional inorganic fillers with the potential to yield composites with improved dielectric properties. Interesting applications for MOF/polymer composites may also exist in the areas of sensors, membranes, and traditional composites (for controlling mechanical, optical, etc. properties).

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