MAR13-2012-020253

Abstract for an Invited Paper
for the MAR13 Meeting of
the American Physical Society

Accelerating Dielectrics Design Using Thinking Machines[1]

R. RAMPRASAD, University of Connecticut

High energy density capacitors are required for several pulsed power and energy storage applications, including food preservation, nuclear test simulations, electric propulsion of ships and hybrid electric vehicles. The maximum electrostatic energy that can be stored in a capacitor dielectric is proportional to its dielectric constant and the square of its breakdown field. The current standard material for capacitive energy storage is polypropylene which has a large breakdown field but low dielectric constant. We are involved in a search for new classes of polymers superior to polypropylene using first principles computations combined with statistical and machine learning methods. Essential to this search are schemes to efficiently compute the dielectric constant of polymers and the intrinsic dielectric breakdown field, as well as methods to determine the stable structures of new classes of polymers and strategies to efficiently navigate through the polymer chemical space offered by the periodic table. These methodologies have been combined with statistical learning paradigms in order to make property predictions rapidly, and promising classes of polymeric systems for energy storage applications have been identified.

[1]This work is being supported by the Office of Naval Research.