Meta-dielectric for energy storage application capacitor

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1. Introduction

Energy storage units having both high energy density and high power density are crucial for further progress of technology. As the limitations of the electrochemical batteries are impossible to overcome, the right answer should arrive from the capacitor side. In the present paper, we propose to use the conjugated polymers with large second-order permittivity to develop capacitors having extremely high energy density. We believe that the proposed approach ushers a new generation of the energy storage devices providing the solutions to the many needs of the society.

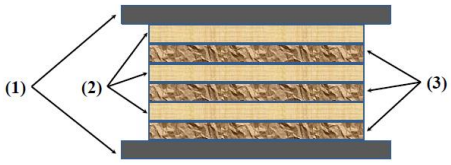

Fig. 1. Alternating layers of material: (1) metallic contacts, (2) high dielectric permittivity layers, and (3) high breakdown voltage materials.

Conjugated polymers are molecular stacks with repeating units of fundamental monomers. While undoped, they are insulators or semiconductors, but with doping they exhibit metallic conductivity. Their polarizability shows a non-linear dependence on the electric field and its magnitude is several orders larger than that of the electronic polarization, especially in the frequency range of kHz-MHz, which makes such systems most suitable for the energy storage purposes because its contribution is the largest at the static fields. The conduction can compromise the high dielectric strength of the dielectric. To avoid this, we propose to couple the aromatic molecules with high polarization to aliphatic alkyl tails. Such combination naturally leads to the layered arrangement, with alternate layers having high permittivity and high breakdown voltage, respectively, as shown in Fig. 1.

2. Second-order permittivity

In this work, we report our analysis of the feasibility to use the nonlinear effects in the polarization of a dielectric based on conjugated polymers. The contributions of the second-order permittivity to the stored energy and to the real part of the dielectric function, as measured in the impedance spectroscopy experiments, are determined. The correspondence of the permittivities and the molecular polarizabilities is established via the generalized non-linear Clausius–Mossotti relations. The expression for the energy density of the proposed heavy-duty capacitor includes the contributions from the first- and second order permittivites, as

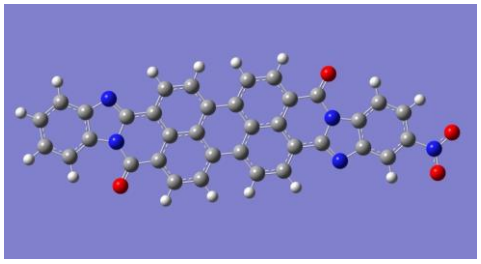

Fig. 2. Nitro-phenyl-perylene molecule with NO_2 group at the apex position.

$$\frac{W}{M} = \frac{1}{3600}\frac{\varepsilon_0}{\rho}\frac{V_{op}^2}{d^2}\left(\frac{\varepsilon^{(1)}}{2} + \frac{2\varepsilon^{(2)}}{3}\frac{V_{op}}{d}\right) \quad (1)$$

where $M = \rho A d$ is the mass of the dielectric, ρ is the mass density, V_{op} is the operating voltage, d is the separation of the capacitor plates, and 1/3600 is the conversion factor from Joules to Watt-hours.

3. Results

We apply our approach to specific nitro-phenyl-perylene (NPP) molecule shown in Fig. 2. A single NO_2 group serving as an electron acceptor is attached at the apex position to introduce a non-symmetric electron density and, correspondingly, large polarizability. We determine the linear polarizability, α, and the hyperpolarizability, β, by means of Gaussian09 quantum chemistry software. We use the B3LYP method with the 6-31G(d)+ basis set. The results are α = 1479 a.u. and β = 18434 a.u. (1 a.u. = $e^2a_0^2/E_h$ for α and 1 a.u. = $e^3a_0^3/E_h^2$ for β, where e is the electron charge, a_0 is the Bohr radius, and E_h is the Hartree energy.) Using generalized non-linear Clausius–Mossotti relations, we calculated the first- and second-order permittivities and substituted them to Eq. (1). The dependence of the energy density on the operating voltage is shown in Fig. 3. One can see from this figure that at high operating voltage this energy density is comparable or can even exceed the values of the current generation of electrochemical batteries.

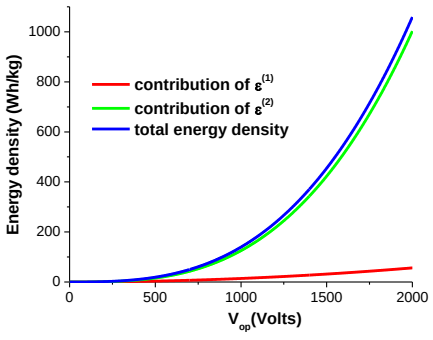

Fig. 3. Energy density of the NPP-based capacitor as a function of the operating voltage.