

Ion Mobility – A Limiting Factor In The Application Of Polypyrrole Actuators.

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Conducting polymers, polypyrrole (PPy) in particular, have been proposed as potential candidates for biocompatible artificial muscle material already some time ago [1]. There have been many studies aiming at the optimal technical setup, solvents, dopant ions, etc. Unlike the case of ion polymer metal composites, the achievable electrochemical stress of conducting polymers is excellent. However, the moderate strain and response rate have hindered the rapid application of such materials as actuators.

The maximum strain and response rate of a conducting polymer film are dependent on the rigidity of the structure of the film and the ion mobility inside, correspondingly. It has been shown previously [2] that the structure of PPy is largely determined by the conditions of the synthesis, and further treatment has only limited effect. The mobility of ions (both cations and anions) is also dependent on the way the polymer film was synthesized (the structure) as well as on the choice of the ions themselves. Therefore, all limiting factors are summed up in ion mobility, which explains why understanding ion mobility in conducting polymer films is of paramount importance.

The results of the comparative study of several small inorganic, as well as slightly larger organic aromatic sulfonate dopant-anions with carefully chosen cyclic voltammetry (CV) measurements together with quantum chemical calculations are presented. The redox charge, influence of the sweep rate, the memory effect, and the mobility of the anions in the polypyrrole films during redox cycling was studied using CV. The geometry and stabilization energies of the (charged and neutral) pyrrole oligomers – anion complexes were studied using a variety of quantum chemical methods ranging from semi-empirical to post Hartree-Fock *ab initio* and density functional theory levels, the methodology that has been used previously for only inorganic anions [3].

The two sets of dopant ions, no matter their similarities, have a surprisingly different effect on the synthesis process and the properties of the polymer film. This variation of the mobility is attributed to two main factors: the steric hindrance and the interaction strength of the anions with the polymer chain. Polymer films of different thickness show remarkably different results, with the thinner films being much more organized. Very interesting results were obtained also from redoping experiments of both organic and inorganic anions. The role and mobility of cations is also assessed.

References.

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