Theoretical study of the PEDOT:PSS/KDP mixture on aqueous medium

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In this work, the interactions between poly(3,4-ethylenedioxythiophene): poly (styrene sulfonate) (PEDOT: PSS) with monobasic potassium phosphate (KDP), a piezoelectric salt, were studied by molecular mechanics and molecular dynamics in aqueous solution. The simulations represent evolutions of previous models, which were part of mechanical and spectroscopic analysis that explained, in part, the electrical behavior of that molecular system. The studied oligomers are long enough, with a minimum of 100 monomers each, in order to allow observation of conformational changes that lead to a better understanding of solvation properties that convert the PEDOT, from insoluble in water to soluble, when complexed with PSS.

Keywords: PEDOT:PSS; KDP; conductive polymers; molecular simulation.

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