PÔSTER - RESUMO - DISPOSITIVOS ELETRÔNICOS, ELETROQUÍMICOS, SUPERCAPACITORES E BATERIAS

INFLUENCE OF WEAKLY COORDINATING SOLVENTS ON ELECTROLYTE PROPERTIES AND SUPERCAPACITOR PERFORMANCE BY MD SIMULATIONS

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Currently, the demand for energy is increasing and is highly relevant to human development. Renewable energy sources, such as wind and solar photovoltaics, are rapidly expanding; however, they exhibit intermittent production. Therefore, it is necessary to couple these sources with energy storage systems to meet demand during nighttime periods and when wind is scarce. [1] Lithium-ion batteries are already well developed, but the natural abundance of lithium is lower compared to sodium, which is more abundant in the Earth's crust. Many efforts have been made to develop efficient and cheaper sodium-ion batteries. [2,3] In this work, we performed molecular dynamics simulations using the LAMMPS program on electrolytes composed of sodium salts in mixtures of propylene carbonate (PC) and cyclopentyl methyl ether (CPME) to investigate transport properties and the characterization of the local structure of bulk electrolytes. In addition, molecular simulations of electrolytes confined in porous carbon electrodes were also carried out to investigate the

electrical properties of electrochemical cells and the structuring of ions within the nanopores of the electrodes under applied voltage. The OPLS force field was used in all simulations. [4] The addition of CPME decreases the viscosity of the electrolytes without increasing conductivity due to the greater formation of ion pairs. Strong Na–carbonate interactions cause solvent molecules to be dragged into the electrode when the negative electrode is filled with Na-cations. In the presence of electrodes and without applied voltage, CPME-rich domains form near the electrode, leading to the formation of NaPF6 and PC-rich domains due to the strong interaction of the salt with PC. Despite this, the charge accumulated in supercapacitors with both salts is similar and agrees with electrochemical experimental data obtained by collaborators from our group.

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Palavras-chave: molecular dynamics; supercapacitor; sodium ion; weakly coordinating solvents.