Enhancing Supercapacitance Through Isomer-Specific Nitroaniline Doping and Heterophase Engineering of Tio2 for High-Performance Supercapacitor

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Abstract:

Novel combinations of inorganic and organic components pave the way for new electrode materials and a better understanding of structure-property relationships. In this work, a simple one-step hydrothermal method was developed to synthesize nitroaniline (x-NA) isomers (x = ortho (o), meta (m), and para (p)) incorporated into TiO_2. The o-/m-/p-NA were incorporated into TiO_2 to enhance capacitance, and phase characterization and optimal structure were found to be critical in determining electrochemical performance. More importantly, o-NA-TiO_2 exhibited the highest specific capacitance (C_s) of 937 F g^{-1} at a current density of 3 A g^{-1}, compared to m-NA-TiO_2 (366 F g^{-1}), p-NA-TiO_2 (559 F g^{-1}), and pristine TiO_2 (411 F g^{-1}). The outstanding performance of o-NA is attributed to the heterophase of anatase and brookite, with the optimal lattice structure and steric hindrance effects. This work demonstrates that precise isomer selection in organic-inorganic hybrid electrode design is a powerful tool for tuning TiO_2 phase composition and lattice architecture, positioning nitroaniline-incorporated TiO_2 as a promising high-capacitance electrode material for next-generation supercapacitors.

Keywords:

Heterophase, mesomeric effect, nitrogen doping, resonance, steric hindrance.