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A MACHINE LEARNING MODEL FOR OPTIMIZATION OF PYRROLE ELECTROPOLYMERIZATION

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Abstract

Pyrrole is a monomer, commonly used for the production of polypyrrole (PPy), a versatile polymer which exhibits multiple useful properties, such as electrical conductivity, resistance to a broad range of pH and temperature conditions. PPy also has a prominent use case in the production of molecularly imprinted polymers, which can further be utilized in electrochemical sensors. However, despite the widespread use of PPy, there have been few attempts to optimize the electropolymerization behaviour using computational modeling. In this paper we present a machine learning model, which is used to optimize the pH and/or buffer choice, upper/lower polymerization voltage for pyrrole electropolymerization using chronoamperometry.

Keywords

Pyrrole, Polypyrrole, Electropolymerization, Machine Learning, Chronoamperometry

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Citations

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