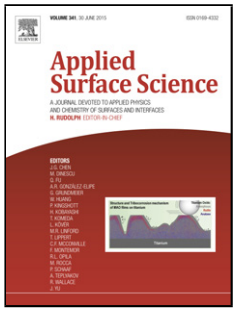

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Characterization of acid functional groups of carbon dots by nonlinear regression data fitting of potentiometric titration curves

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Abstract

The oxygenated functional groups present on the surface of carbon dots with an average size of 2.7 ±0.5 nm were characterized by a variety of techniques. In particular, we discussed the fit data of potentiometric titration curves using a nonlinear regression method based on the Levenberg Marquardt algorithm. The results obtained by statistical treatment of the titration curve data showed that the best fit was obtained considering the presence of five Brønsted-Lowry acids on the surface of the carbon dots with constant ionization characteristics of carboxylic acids, cyclic ester, phenolic and pyrone-like groups. The total number of oxygenated acid groups obtained was 5 $mmolg^{-1}$, with approximately 65% (~2.9 $mmolg^{-1}$) originating from groups with pKa <6. The methodology showed good reproducibility and stability with standard deviations below 5%. The nature of the groups was independent of small variations in experimental conditions, i.e. the mass of carbon dots titrated and initial concentration of HCl solution. Finally, we believe that the methodology used here, together with other characterization techniques, is a simple, fast and powerful tool to characterize the complex acid-base properties of these so interesting and intriguing nanoparticles.

Keywords: nanostructures, oxidized carbon dots, acids functional groups, potentiometric titration, electrochemical techniques and nonlinear regression.

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