Acid-free hydrothermal-extraction and molecular structure of carbon quantum dots derived from empty fruit bunch biochar

ABSTRACT

Carbon quantum dots (CQD) have great potential to be used in various applications due to their unique electrical and optical properties. Herein, a facile, green and eco-friendly hydrothermal method for the preparation of carbon quantum dots was achieved using empty fruit bunch (EFB) biochar as a renewable and abundant carbon source. In the current study, the role of the hydrothermal process was observed and studied by comparing the morphology and optical characteristics of CQD obtained from EFB biochar. Interestingly, based on the high-resolution transmission electron microscopy (HRTEM) result, a considerably similar carbon quantum dots structure can be observed for the EFB biochar sample, showing the similar size and distribution of CQD. To further discuss the extraction of CQD from EFB biochar, a mechanism based on hydrothermal-induced extraction of CQD is proposed. The optimal structure of CQD deduced by density functional theory (DFT) in energy and dipole momentum was about 2057.4905 Hatree and 18.1699 Debye, respectively. This study presents a practical experimental approach in elucidating the molecular structure of photoluminescence CQD based on the Fourier transform infrared (FTIR) spectroscopy, X-ray photoelectron spectroscopy (XPS) and transmission electron microscopy (TEM) results.

Keyword: Carbon quantum dots; Empty fruit bunch; Hydrothermal; Extraction; Photoluminescent; DFT