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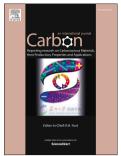
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Direct Photodissociation of toluene molecules to Photoluminescent

Carbon Dots under Pulsed Laser irradiation

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Abstract:

Herein, we report a facile method of direct photodissociation of toluene molecules to

photoluminescent carbon dots (CDs) under pulsed laser irradiation in the absence of

surfactants or catalysts. The as-synthesized CDs with diameters 1.3-4.0 nm present

regular emission peaks and the crystallographic structure of these species has been

identified as graphite 2H from the analysis of high resolution transmission electron

microscope (HRTEM) images, X-ray photoelectron spectroscopy (XPS) and Raman

spectrum. In addition, First-Principle calculations were performed to discuss the

photon-induced excitation in the photodissociation processe. The results demonstrate

that electrons can be transited from Highest Occupied Molecular Orbital (HOMO) to

Lowest Unoccupied Molecular Orbital (LUMO) in toluene molecule by 248 nm

single photon excitation processe and the Stark effect plays a crucial role in the

photodissociation processe. These CDs exhibit excellent stable emission due to the

stability of crystal structure, which could be considered for promising luminescent

applications.

1. Introduction

Carbon nanomaterials have a broad range of applications in energy, environmental

and biomedical fields [1-6]. In particular, photoluminescent carbon dots (CDs)

including graphene dots (GDs) have received considerable interests due to their

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