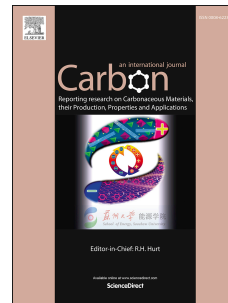


# Accepted Manuscript

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PII: S0008-6223(16)30951-4

DOI: [10.1016/j.carbon.2016.10.089](https://doi.org/10.1016/j.carbon.2016.10.089)

Reference: CARBON 11435

To appear in: *Carbon*

Received Date: 12 July 2016

Revised Date: 5 October 2016

Accepted Date: 29 October 2016

Please cite this article as: F. Gao, S. Ma, J. Li, K. Dai, X. Xiao, D. Zhao, W. Gong, Rational design of high quality citric acid-derived carbon dots by selecting efficient chemical structure motifs, *Carbon* (2016), doi: 10.1016/j.carbon.2016.10.089.

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# Rational design of high quality citric acid-derived carbon dots by selecting efficient chemical structure motifs

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## Abstract

A green pyrolysis approach to prepare ultra-small nitrogen and sulfur-co-doped carbon dots (N,S-C-dots, QY reaches 55.7%) with precursors citric acid (CA) as carbon source and N-acetyl-L-cysteine as N and S dopant has been explored. The optical properties and the origin of photoluminescence (PL) have been investigated at length. The excitation independence character ( $200 \leq \lambda_{\text{ex}} \leq 380$  nm) and the excitation dependence feature ( $\lambda_{\text{ex}} > 380$  nm) along with the biexponential behavior of lifetime of prepared C-dots all indicate the existence of two different emissive sites: the surface state caused by the introducing of N and S on C-dots surfaces and the molecular state induced by the fluorophores covalently bonded onto C-dots surfaces. More importantly, for the first time, through comprehensively comparing the PL performances of various types of N,S-C-dots, N-C-dots and S-C-dots synthesized under same condition, we report the efficient chemical structure motif of reactant, which could form small fluorophore molecules with high PL during the synthesis and thus exhibits favorable impact on PL performances of resulting C-dots. Detailed structural and property studies suggest that the chemical structure motif of reactant ( $-\text{HN}-\text{C}-\text{C}-\text{SH}$ ) determines the optical properties of CA-derived C-dots, which would be valuable in selecting efficient reactants for preparing highly fluorescent CA-derived C-dots.

Keywords: Carbon dots, synthesis, photoluminescence mechanism, chemical structure

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