***Research Article***

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# The investigation of cavity-trapped electrons in the $Na_n$@Tetracyanoethylene (n=1-4) systems

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ABSTRACT

Electride materials are very interesting that have cavity-trapped electrons. In different systems, this materials can be used as source of electron donor. Hereby, we have explored the possible of electride materials based on tetracyanoethylene (TCNE) backbone, computationally. This is achieved through the addition of up to four Na-atoms to the TCNE backbone. Our results in this work, predict high thermodynamic stability for the $Na_n$@TCNE (n=1-4) systems. Also, based on the evaluation of four criteria, non-nuclear attractor (NNA), electron localization function (ELF), electron density laplacian ($\nabla^2\rho(r)$), and non-linear optical (NLO), TCNE-$Na_1$ and TCNE-$Na_2$ and TCNE-$Na_4$ species are lithium salt. In contrast, the TCNE-$Na_3$ species can be introduced as sodium electride with cavity-trapped electrons. Therefore, Na:TCNE ratio is very significant factor to provide species with electride feature through the addition of Na atoms to TCNE backbone.

## 1.Introduction

Materials with electride property have achieved much attention in the recent years. The history of the electride materials begins by the introduction of alkali metal-ammonia solutions and solvated electrons in solution [1]. In addition, the first to postulate the existence of electrides, synthesize and characterize them was Dye et al [2-8]. The electrides (with cavity-trapped electrons) can be introduced as the smallest possible anions [9].

Note that the confined electrons in the electride do not belong to any specific atom. It is interesting to notice that the electrides have low work function. Therefore, they can be used as strong reducing agents in chemistry. Unique properties of electrides can provide suitable opportunity for researchers to study electron transfer process at room temperature. Moreover, the isolated electrons in the electrides cause its potential applications such as the improved cathode material for fluorescent lights [10], emitting diodes for organic light [11], improved catalysts for the $CO_2$ activation [12], splitting of $N_2$ molecule [13-15], storage device of $H_2$ molecule with reversible features [16] and powerful and selective reducing agents [17-19].

In the electride materials, the density of the confined electrons is not big enough to identify through the X-ray. Therefore, experimental researchers used indirect evidence [20-22] to achieve its experimental characterization. Indeed, a few researchers have attempted to analyze the electronic structure of the electrides [23, 24]. This means that computational techniques can be more suitable tools to identify the electride materials. In this regards, researchers used different computational techniques to identify the electride material. For example, some researchers introduced materials as electride based on large non-linear optical properties (NLO) [25-27], non-nuclear attractors (NNAs) [28, 29] and electron localization

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