

# Investigation of hydrogen adsorption and storage on G-C<sub>3</sub>N<sub>4</sub>: fuel cell application

Siroos Rostami<sup>\*</sup>, Ali Nakhaei Pour, Hasan Oliaei Torshizi

Department of Chemistry, Faculty of Science, Ferdowsi University of Mashhad, Iran

#### ARTICLE INFO:

Received: 3 December 2019

Accepted: 4 April 2020

Available online: 10 April 2020

⊠: S. Rostami Siroosrostami90@gmail.com

### ABSTRACT

In this paper we experimentally worked on hydrogen storage on G-C<sub>3</sub>N<sub>4</sub> in ambient temperature and 20 bar pressure. Also we determined thermodynamical properties of hydrogen adsorption. We synthesized pure G-C<sub>3</sub>N<sub>4</sub> by Urea Precursor and it proved by XRD and FT-IR spectra. Results show that the pure G-C<sub>3</sub>N<sub>4</sub> adsorption isotherm matched to Freundlich adsorption isotherm and  $\Delta H_{ad}$ ,  $\Delta G_{ad}$  and  $\Delta S_{ad}$  obtained about (-27 kj/mol), (+21 kj/mol) and (-161 j/k) respectively. Result showed pure G-C3N4 have low hydrogen storage and could not consider as candidate for hydrogen storage materials and must equip with other materials like metal oxide, transitional metal and to promote capacity of G-C<sub>3</sub>N<sub>4</sub> compounds for fuel cell application.

*Keywords*: Hydrogen; G-C<sub>3</sub>N<sub>4</sub>; Storage

# **1. Introduction**

Carbon compounds have been considered as candidate for hydrogen storage because of lightweight, porosity and etc. nowadays researchers have been attempted to modify the structure of carbon compounds to enhance hydrogen storage. G-C3N4 considered as some of these materials which have higher hydrogen storage than similar activated carbon. Researchers attributed these properties to presence of C-N bonds instead of C-C bonds increase hydrogen storage [1-3].

#### 2. Experimental

#### 2.1. Materials and Methods

G-C<sub>3</sub>N<sub>4</sub> has been synthesized by urea precursor like each preparation methods have been observed elsewhere [4]. For experimental preparation G-C<sub>3</sub>N<sub>4</sub> we used Urea precursor, were purchased from Merk as received without additional purification. We put crucible with Urea in furnace and raised temperature to 550°C step by step (4 step in hour) and hold this circumstance for 2 hours at last we observed yellow G-C<sub>3</sub>N<sub>4</sub> product. Previous processes yielded yellow product then milled and made pellet and put 1.5 gr in sample tube then checked out apparatus from gas leaking. G-C<sub>3</sub>N<sub>4</sub> was proved by FT-IR, XRD spectra and specific surface area obtained (SBET =  $27 \text{ m}^2/\text{gr}$ ). Hydrogen adsorption carried out by homemade volumetric adsorption apparatus and system checked for leaking presence. Also we carried out adsorption processes in different temperatures to find thermodynamical parameters.

#### 3. Results and discussion

For finding thermodynamical properties we used Equation 1 so hydrogen storage of substrate obtained in different temperature had been showed in Fig.1 and  $\Delta H_{ad}$  calculated.

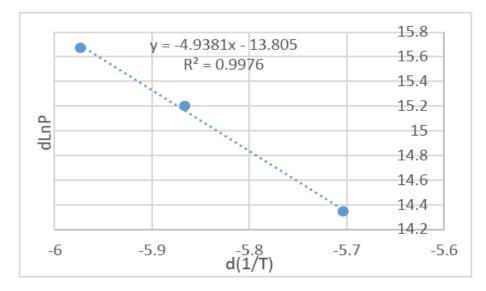


Fig.1: Hydrogen adsorption in different temperature

 $dLnP/d(1/T) = \Delta H_{ad}/R$  Eq.1

In this experiment we obtained  $\Delta H_{ad}$ , about -28 kJ/mol.

Also we obtained adsorption capacity of  $G-C_3N_4$  substance and evaluated the Langmuir, Temkin and Freundlich isotherms. Results show that the hydrogen adsorption on  $G-C_3N_4$ have better adjustment by Freundlich adsorption isotherm, (Fig.2-4) presented as follow:

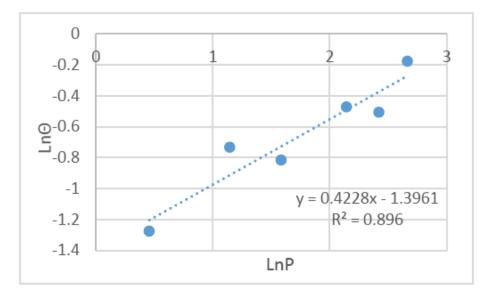


Fig.2: Freundlich isotherm

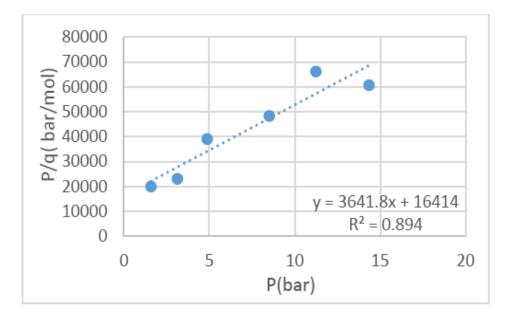


Fig.3: Langmuir isotherm.

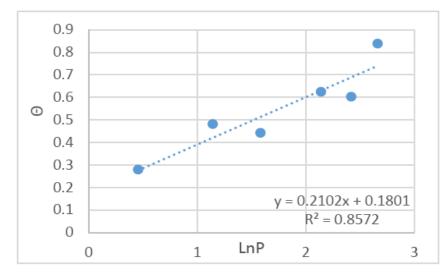


Fig. 4. Temkin isotherm

According to equation 2 and 3 we be able to find thermodynamical properties.  $Q_m$  is amount of monolayer of hydrogen molecules adsorbed on adsorbent surface and  $b_L$  is Langmuir constant.

 $\Delta G = \Delta H - T \Delta S \qquad Eq.2$  $\Delta G = -RT \ Lnb_L \qquad Eq.3$ 

Table 1: Thermodynamic parameters

$\Delta G_{ad (kJ)}$	$\Delta H_{ad~(kJ)}$	$\Delta S_{ad (J/K)}$	$Q_m \ (mmol/gr)$	b <sub>1 (1/bar)</sub>
+21.014	-27.360	-161.24	0.2745	2.1619*10-4

## 4. Conclusions

United States of department of energy (USDOE) aimed finding Adsorbent with 7.5 wt%  $H_2$  storage capacity until 2020. Also G-C<sub>3</sub>N<sub>4</sub> considered carbon material for hydrogen storage because of lightweight but our studies showed pure G-C<sub>3</sub>N<sub>4</sub> cannot be reliable adsorbent and it is necessary to modified with other materials to enhance G-C<sub>3</sub>N<sub>4</sub> hydrogen capacity to reach USDOE target.

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