Supporting Information

Facile synthesis of NiS$_2$ nanoparticles ingrained in sulfur-doped carbon nitride framework with enhanced visible light photocatalytic activity: Two functional roles of thiourea

Milad Jourshabani,[a,b] Zahra Shariatinia,*[a] Gopal Achari,[b]

Cooper H. Langford[c] and Alireza Badiei[d]

[a]*Department of Chemistry, Amirkabir University of Technology (Tehran Polytechnic), P.O.Box:15875-4413, Tehran, Iran. *E-mail: shariati@aut.ac.ir.*
[b]*Department of Civil Engineering, University of Calgary, 2500 University Drive NW, Calgary, AB, Canada.*
[c]*Department of Chemistry, University of Calgary, 2500 University Drive NW, Calgary, AB, Canada.*
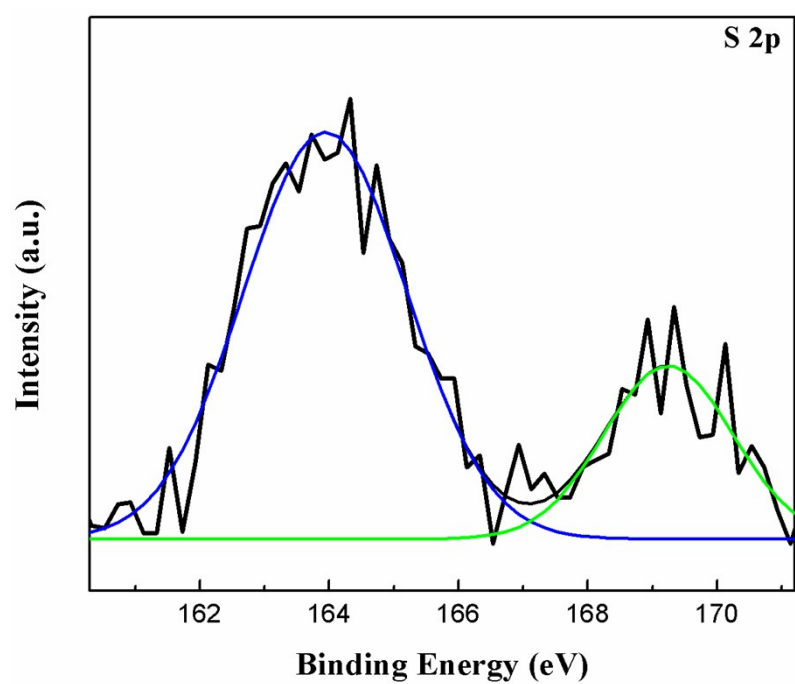[d]*School of Chemistry, College of Science, University of Tehran, Tehran, Iran.*

Fig. S1 The high-resolution XPS spectrum in the S 2p region for the NiS$_2$(5.9)/CNS nanocomposite.

Compound	ESP	Contour map
1		
2		
3		
4		

Fig. S2 The electrostatic surface potentials (ESPs) and contour maps for
the pure carbon nitride (CN, **1**) and its three S-doped CN (**2-4**) compounds
computed at B3LYP/6-31G(d,p) level of theory in water.
Red and yellow colors represent negative and positive regions of the wave functions, respectively.
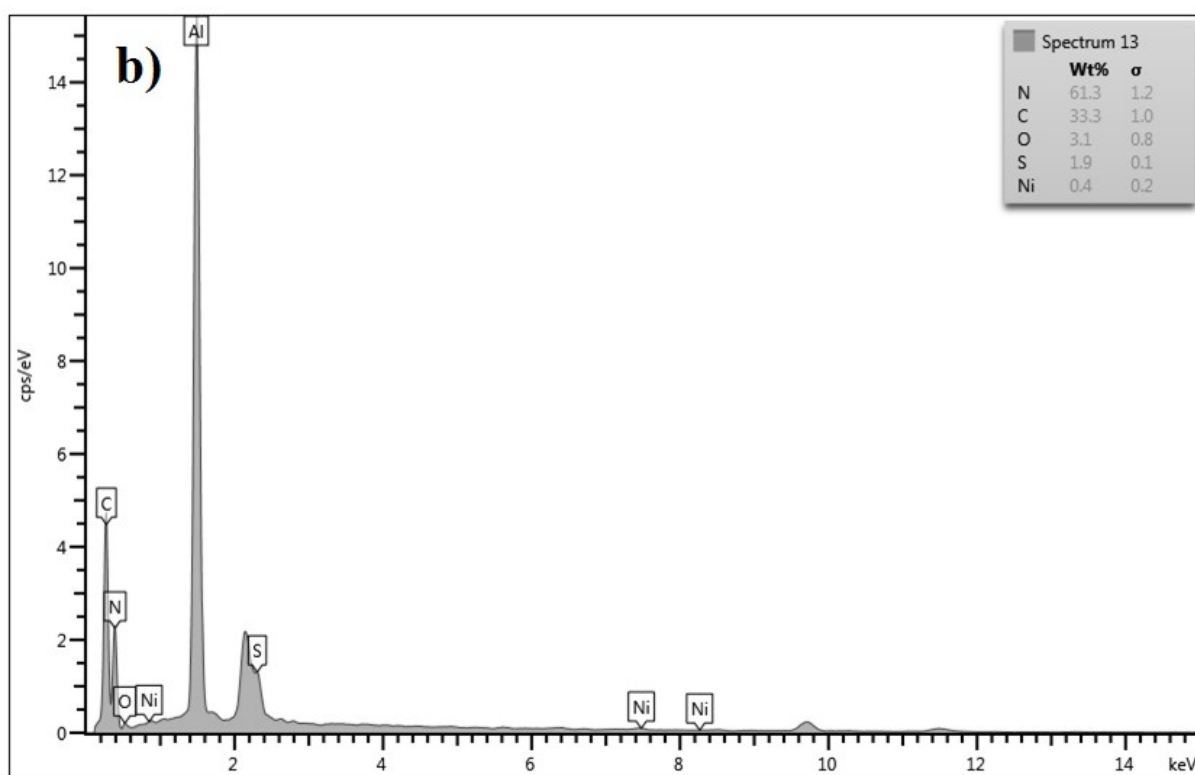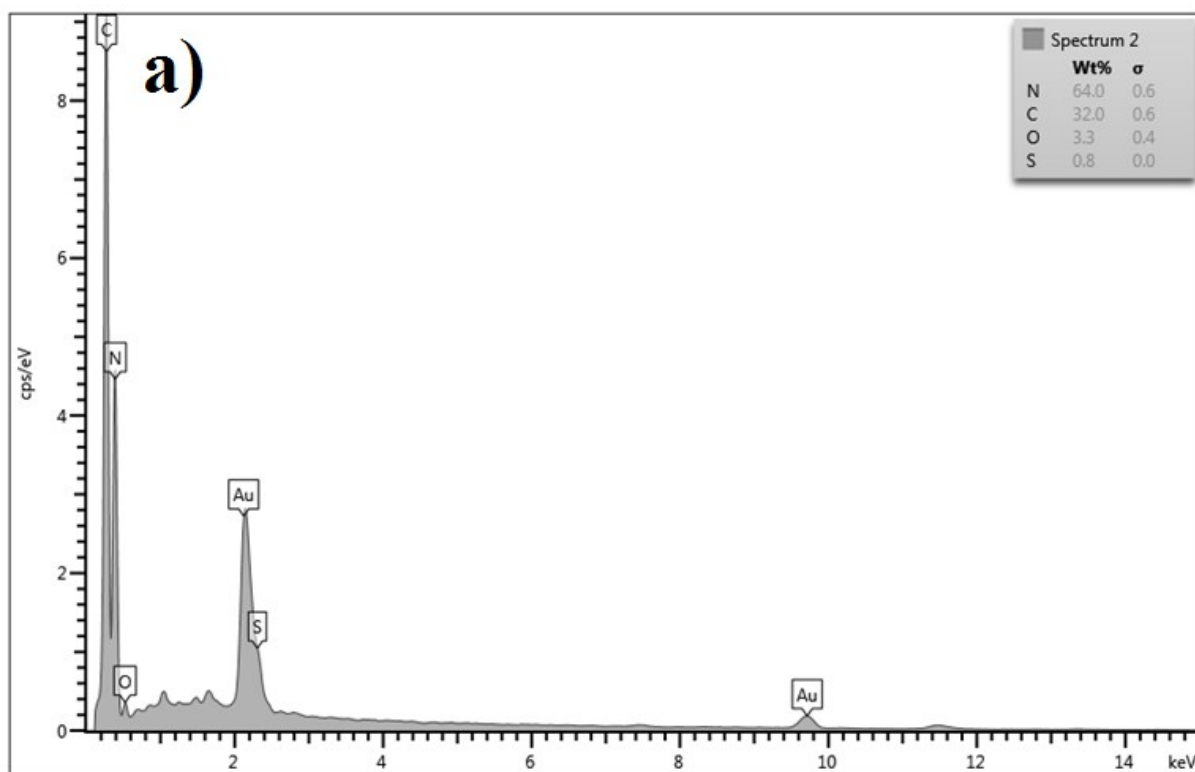
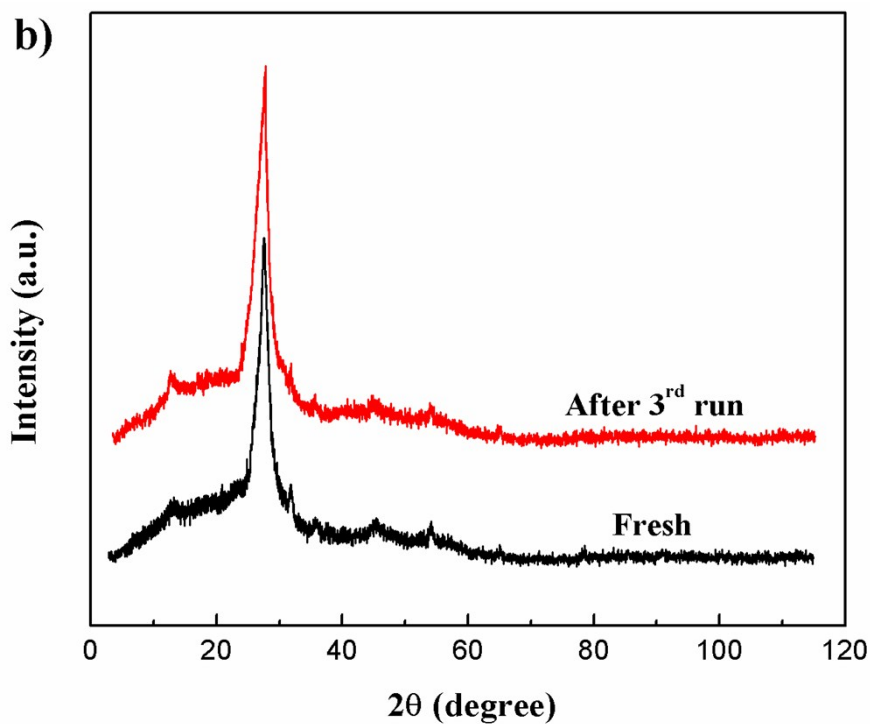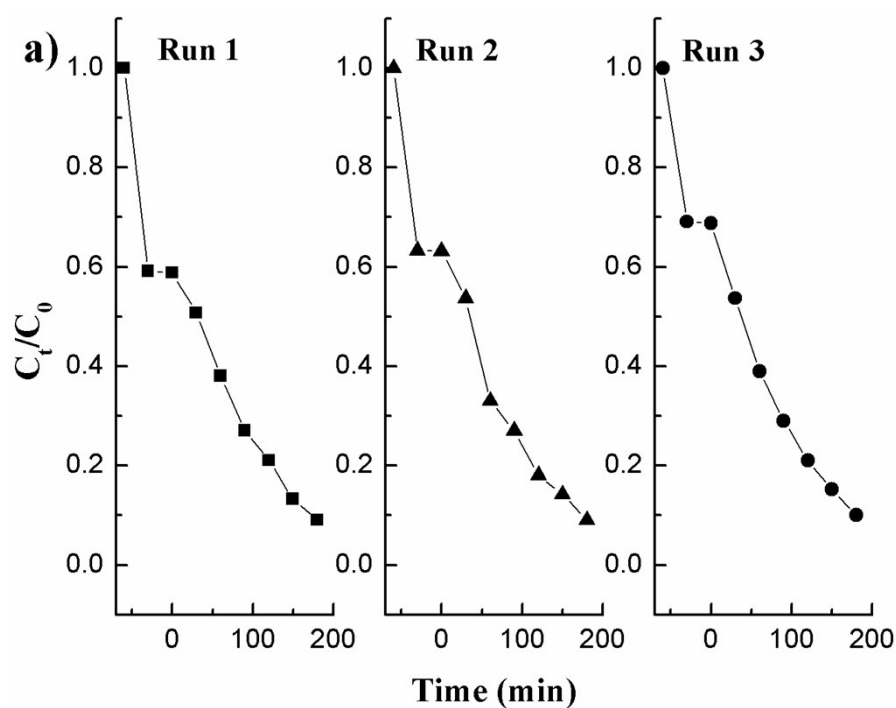**Fig. S3** The EDX plots for the (a) CNS and (b) $NiS_2(5.9)/CNS$ samples.

Fig. S4 (a) Recyclability of the NiS$_2$(5.9)/CNS photocatalyst used in three experiments

for the photocatalytic degradation of RhB under visible light irradiation and

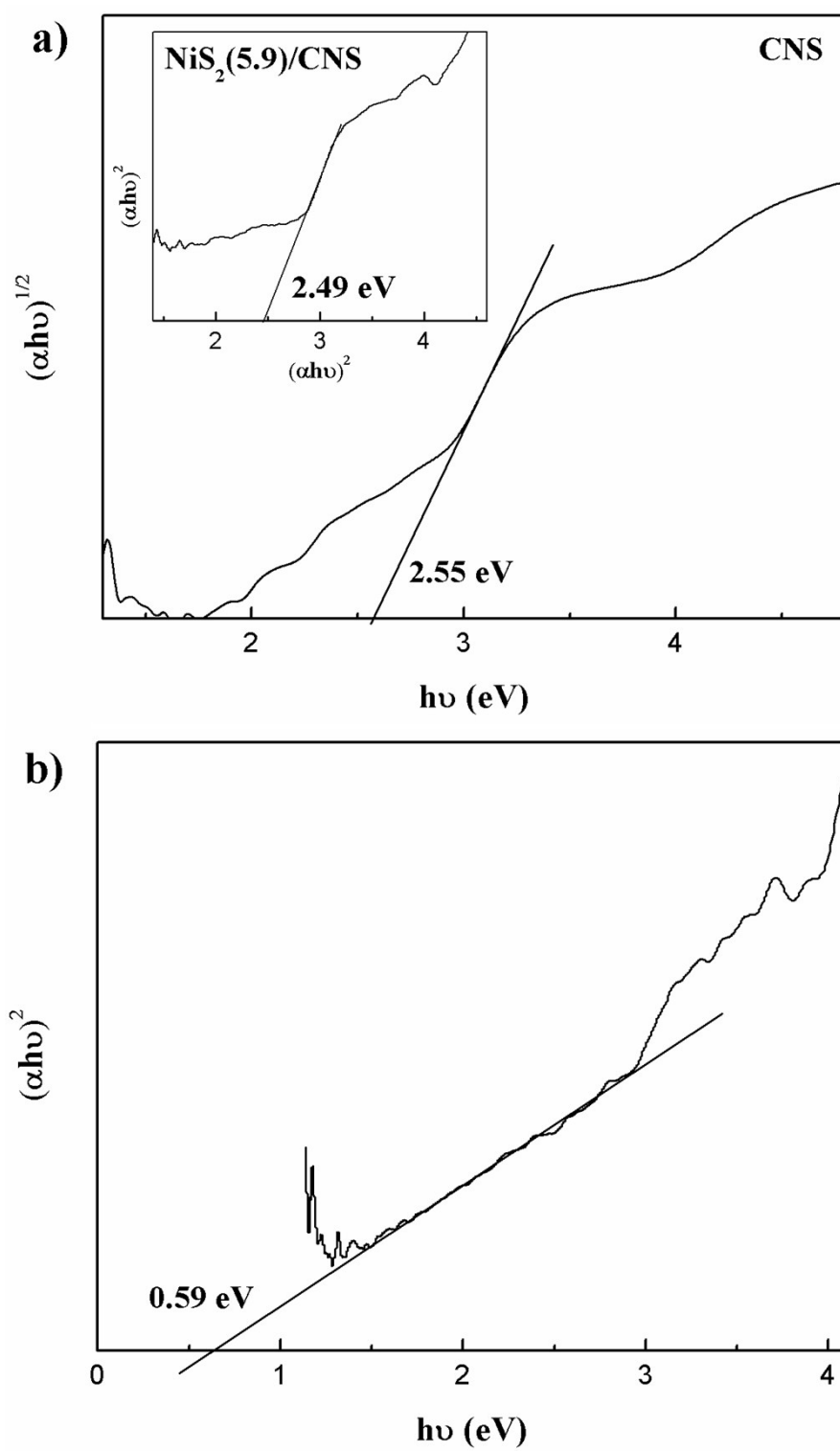(b) the XRD patterns for the NiS$_2$(5.9)/CNS sample before and after the cycling photocatalytic experiments.

Fig. S5 The Tauc plots for (a) CNS and $NiS_2(5.9)/CNS$ and (b) NiS_2 samples.
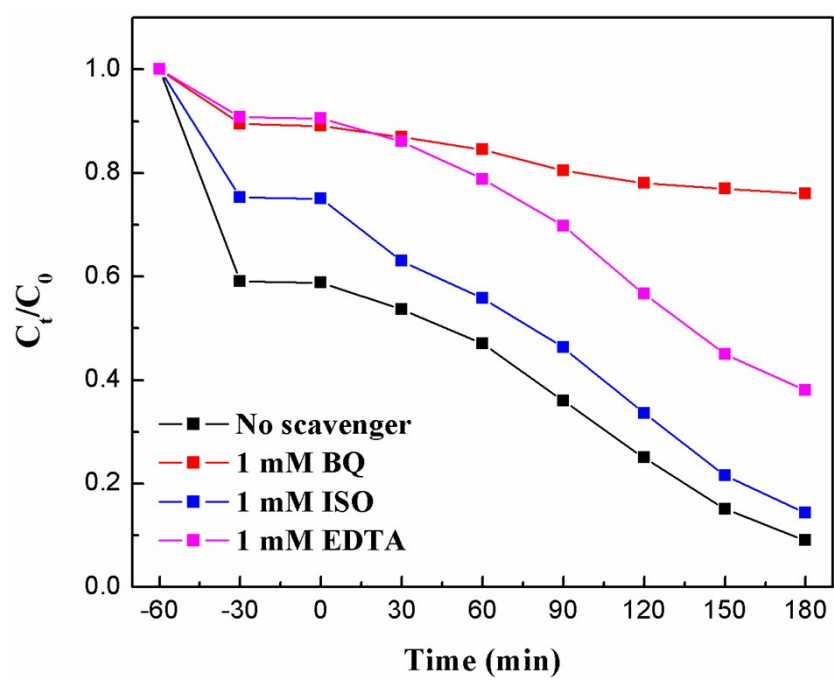
Fig. S6 Influence of various trapping agents on the RhB catalytic degradation
in presence of the NiS$_2$(5.9)/CNS composite photocatalyst.