Evaluation of *N*-doped graphene role in the photodegradation of sulfamethoxazole

A Urda[1,2], C Socaci[1], T Radu[1], V Floare-Avram[1], D Cosma[1] and M C Rosu[1]

[1]*National Institute for Research and Development of Isotopic and Molecular Technologies, Donat 67-103, RO-400293 Cluj-Napoca, Romania*

[2]*Faculty of Chemistry and Chemical Engineering, Department of Chemistry and SOOMCC, Babes-Bolyai University, 400028 Cluj-Napoca, Romania*

Sulfamethoxazole is an emerging contaminant that is found in surface waters. In this study we followed its removal by means of adsorption and photocatalysis processes using materials based on N-doped graphene/TiO_2. These processes were monitored using liquid chromatography (HPLC, on a C18 column). The photocatalytic activity of the prepared materials was performed under UVA light (320-400 nm) and cold white light (420 – 800 nm) using a Luzchem LZC-4V photoreactor.

Preparation of TiO_2Ag-NGr

GO powder dispersed in water + **melamine**

sonicated for 100 minutes

resulted suspension was stirred at 160°C for 8 hours, in an autoclave

black suspension

sonicated for 60 minutes

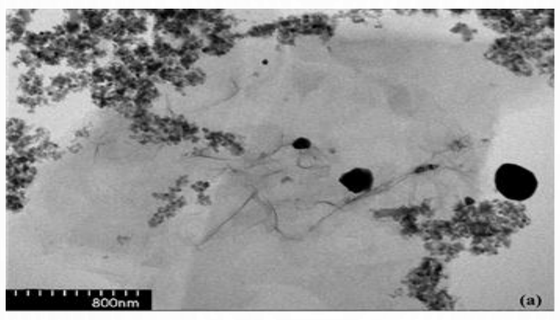
mixed with TiO_2Ag in water

thermally treated at 650°C for 60 minutes

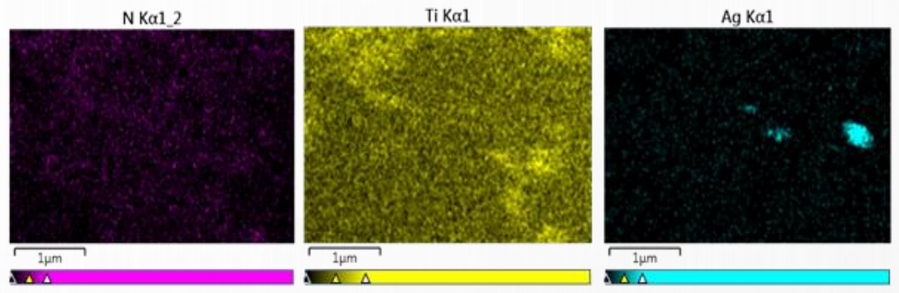
TiO_2Ag-NGr

Characterization

Morphological characterization of the TiO_2Ag-NGr composite

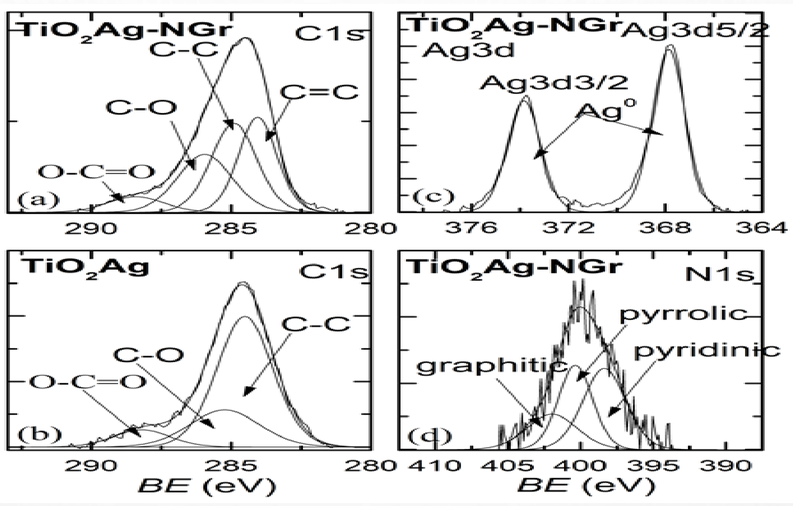


TEM image of TiO_2Ag-NGr (bar = 50 nm).



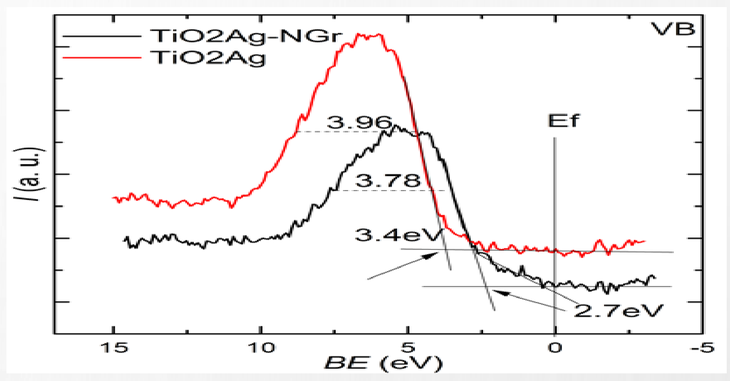
Element mapping images of TiO_2Ag-NGr revealing the distribution of N (magenta), Ti (yellow) and Ag (cyan) elements and the corresponding EDX spectrum.

Structural properties of TiO_2Ag-NGr



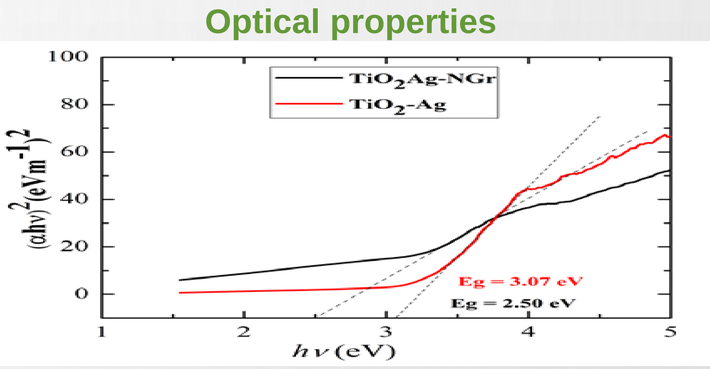
C1s spectra (a and b), Ag3d (c) and N1s spectra (d) for the investigated samples.

Photoelectronic properties



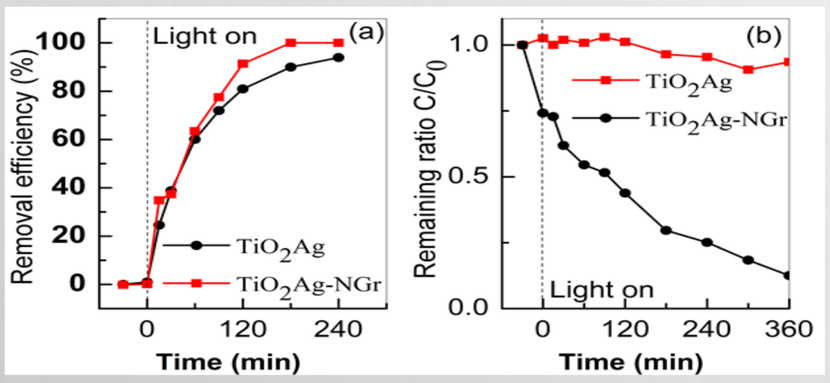
VB XPS valence band spectra of TiO_2Ag (red line) and TiO_2Ag-NGr (black line).

Optical properties



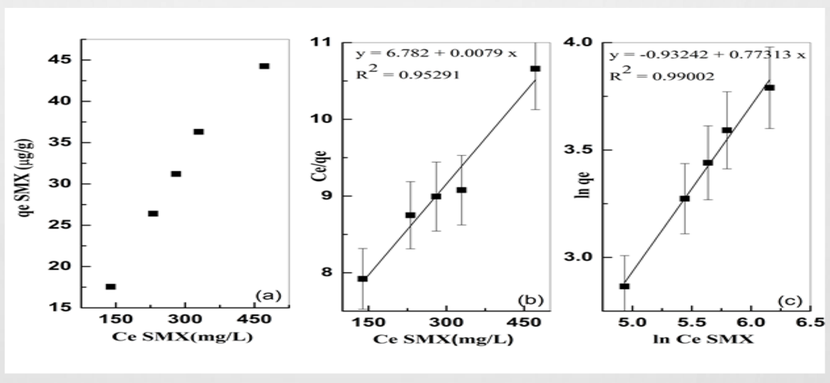
Tauc plots of TiO_2Ag-NGr and its precursor, TiO_2Ag.

Photocatalytic performance in the degradation of sulfamethoxazole

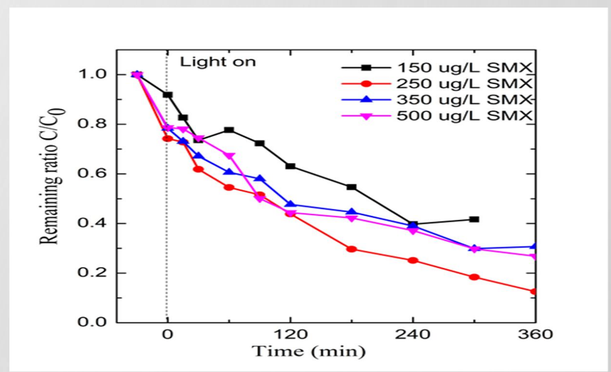


I. UVA light-induced SMX photodegradation for the studied catalysts
II. SMX photodegradation with visible light - Comparison of TiO_2Ag photocatalyst with or without nitrogen-doped graphene.

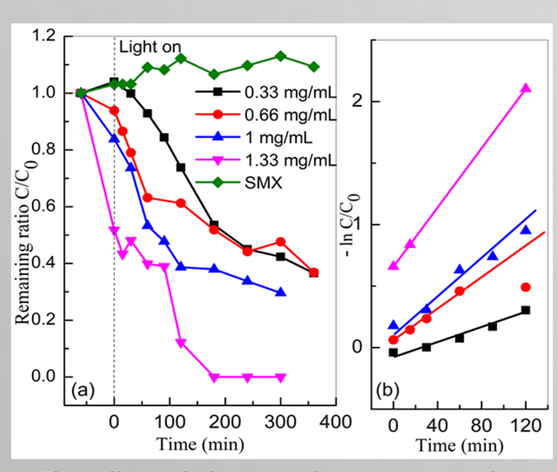
The effect of initial SMX concentration



I.Adsorption isotherms of sulfamethoxazole onto TiO_2Ag-NGr.
II. The Langmuir linearization fit for adsorption of SMX on TiO_2Ag-NGr.
III. The Freundlich linearization fit for adsorption of SMX on TiO_2Ag-NGr.

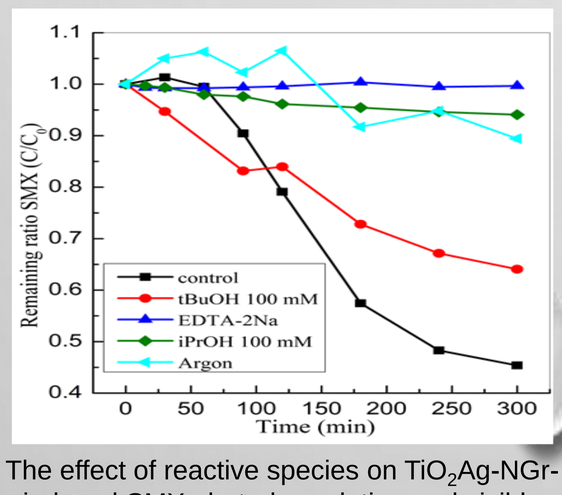


The effect of initial sulfamethoxazole (SMX) concentration on the photodegradation process.

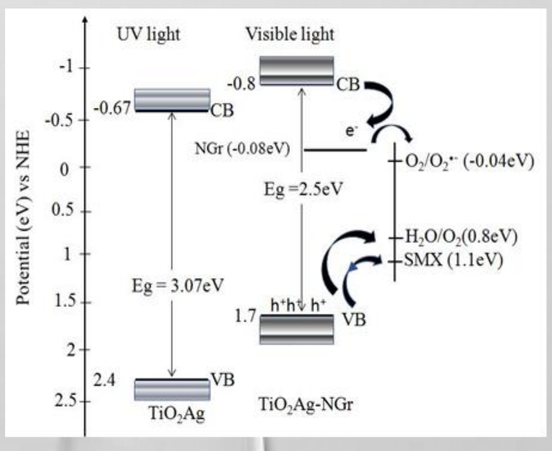


I.The effect of photocatalyst concentration on the adsorption / photodegradation process of SMX in the presence of visible light (II) 1st order kinetics.

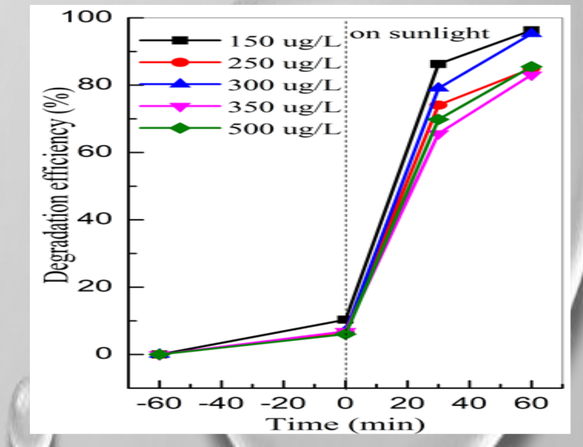
Reactive species and mechanistic considerations



The effect of reactive species on TiO_2Ag-NGr-induced SMX photodegradation and visible light.



Band edge positions of studied photocatalysts relative to the energy levels of the redox couples involved in the oxidation of SMX.



One hour sunlight photodegradation of SMX (different concentrations) with TiO_2Ag-NGr.

CONCLUSIONS

VB XPS and UV-Vis spectroscopic results evidenced that its presence in the composite led to a narrower band gap energy of TiO_2Ag-NGr to 2.5 eV compared to 3.07 eV obtained for the TiO_2Ag material and consequently to the extension of the photocatalytic ability towards the visible light region. The results of the adsorption/photodegradation investigation indicated a very good efficiency in the optimized experimental conditions and under sunlight exposure. The experimental tests for the involved reactive species confirmed the role of the graphene doped with nitrogen as electron capturer in the composite, which is essential in the photocatalytic mechanism.

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