Discovery of a new photocatalyst to solve water pollution

Entry to the Junior Water Prize 2019

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Abstract

My project deals with heterogenic phocatalysis. Photocatalysis is a process, where specific substances called photocatalysts absorb radiation and the results produce radicals . These radicals are ions which can eliminate unwanted organic and anorganic pollutants (unwanted substances which pollute water).

The best property of photocatalysts is that they are absolutely unobjectionable, because the product between radicals and pollutants is clean water.

Nowadays, there are photocatalysts which absorb wavelengths of UV radiation and produce radicals which effectively eliminate pollutants. The most famous is titanium dioxide (TiO_2). Although TiO_2 is the most famous photocatalyst, it can produce radicals only when it absorbs wavelengths of UV radiation. It is not useful if we want clean large areas of rivers. We need UV lamps to produce UV radiation and it would be very expensive. Although there is an amount of UV radiation in light emitted from the Sun it is still not enough for the photocatalytic process to take place.

Because of it, I decided to find the photocatalyst which would be able to produce radicals after absorbing wavelengths of visible light.

I used quantum chemistry software and finally found graphitic carbon nitride: g-C_3N_4 (form B). After cooperation with scientists from Greece who helped me synthetize g-C_3N_4 (form B) I continued my experimental work in the lab.

The efficiency of g-C_3N_4 (form B) was investigated by using UV/Vis spectrometry. The results showed that graphitic nitride has amazing properties and can clean polluted rivers in the world.

This can be obtained by using a very simple method: We can just sprinkle g-C_3N_4 (form B) into rivers and wait for the results which means clean water.

List of abbreviations and acronyms

AM1	Austin Model 1	HCH	Hexachlorocyclohexane
AOP	Advanced Oxidation Processes	HOMO	Highest occupied molecular orbital
DCIP	2,6- Dichlorophenolindophenol	LUMO	Lowest occupied molecular orbital
DDT	Dichlorodiphenyltrichloroethane	MB	Methylene blue
e^-	Electron	MM	Molecular Mechanics
eV	Electronvolt	MO	Molecular Orbital
g-C_3N_4	Graphitic carbon nitride	nm	nanometer
h+	Positive hole	UV / Vis	Ultraviolet / visible
$O_2^{\bullet-}$	Superoxide anion radical	Vis	Visible
$OH^{\bullet}$	Hydroxyl radical	ZnO	Zinc oxide
SW	Software	ΔE	Banned energy chain width
TiO_2	Titanium dioxide		
UV	Ultraviolet		
(D, H, C, P)	Dye, Herbicide, Colour, Pesticide		

My story

My name is Diana Virgovicova. I am 17 years old. I am from Slovakia but currently study at Francis Holland School in London, England.

I have had a passion for chemistry and especially physical chemistry since I was 5 years old. I always wanted to achieve something amazing, something which could make human lives easier and of course change the world. I was often thinking about scientific topics and wanted to work on research. I know that working on projects would teach me more than I could learn in school.

I am very interested in environmental problems. I have read that rivers in the world are very polluted. When I was in India I saw black rivers. There I realized that pollution is enormous.

I started to think about a solution for this problem and chased a link to the best Slovak university where I independently started to work on the first research in my life.

I found an amazing topic dealing with my love for environmental problems, chemistry and physical chemistry all in one unit. I found heterogenic photocatalysis. At the beginning, it was very difficult and I had no idea what to do. Modern photocatalysis is focused on quantum chemistry- which means using diverse computer software for the prediction of properties of substances and courses of photocatalytic reactions. I needed to learn how to work with this software.

After challenging myself to four months of continuous learning I found it easier. I remember clearly - on a very cold day in winter - I found my idea: If I know how to use this software and understand photocatalysis, I can try to find a photocatalyst which will have such properties that can produce radicals by using wavelengths of visible light.

After this I read many books about photocatalysis and I found that a substance called graphitic carbon nitride has better properties than other photocatalysts, but still doesn´t work in the range of wavelengths of visible light.

I transferred an excisting graphitic carbon nitride structure (form A) to a new structure – form B. Form B seemed to have better properties for photocatalysis than all well-known photocatalysts. And it was also confirmed by my quantum chemistry calculations.

I asked scientist from Greece who work at Institute Demokritos in Greece, if they could synthetize this compound for me.

Scientist who also work research heterogenic photocatalysis was amazed. He immediately told me that he has never seen such amazing properties as my graphitic carbon nitride has.

A few days later, scientists from Greece synthetized g-C3N4 (form B) by annealing melamine at 650°C and sent it to me. I was very excited, I could continue working on my research, but now experimentally in a lab. I needed to learn how to work with a UV/Vis-spectrometer and also find which pollutants would be the best for my experiment. But finally in June 2018 my experiments showed that g-C3N4 (form B) is as amazing as I had hoped.

Every experiment confirmed that g-C3N4 (form B) has a bright future in cleaning rivers and saving human lives all around the world.

Following my academic results from my school in Slovakia, I got one of the biggest opportunities of my life, I won 100% scholarship for studying in the UK, where I continued with my project. I improved my theoretical understanding and completed further calculations to confirm my results.

My project contains calculations which are absolutely original; calculations of optical transfer and oscillator power by using very new method of Zindo/S for AM1.

I am delighted to have the opportunity to share my work as part of the Junior Water Prize in Stockholm.

Acknowledgements

I wish to express my sincere gratitude to Proffesors from Slovakia for providing me an opportunity to work on the first scientific research of my life at The Faculty of Chemical Technology in Bratislava.

I sincerely thank to the scientists from Greece (Institute of Demokritos, Athens, Greece) who synthetized my newly designed modification of g-C_3N_4.

I would like to thank to my family, my brother and my sister who taught me how to use quantum chemistry software.

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1 Introduction

This project aims to develop a new working solution for the growing problem of river pollution. The work deals with the experimental and theoretical study of the degradation of the 2,6-dichlorindophenol (DCIP) model compound with a newly synthetized and proposed photocatalysts based on boron and nitrogen atoms (g-C3N4). This new photocatalyst was predicted and developed using quantum chemistry software, before testing a synthesised sample using UV/Vis spectrometry to measure its effectiveness as a photocatalyst to produce radicals, which can then eliminate unwanted organic and inorganic chemical pollutants. The changes in the optical spectra of the DCIP/g-C3N4 aqueous suspension were monitored by discontinuous UV radiation with a wavelength of 365 nm and visible radiation at a wavelength of 405 nm. The experiments showed that the minimum effect of photodegradation was observed for the wavelength at 405 nm, visible radiation, which indicates the potential for a significant improvement in the use of photocatalysts to combat river pollution.

2 Materials and methods

When I was in India I saw black rivers, there I realized that pollution is enormous…

Currently, more and more pollutants accumulated in the soil, in the air or in the water, are getting into the environment with devastating long term consequences. Environmental protection must now, without delay, be a top priority for international political and scientific collaborations.

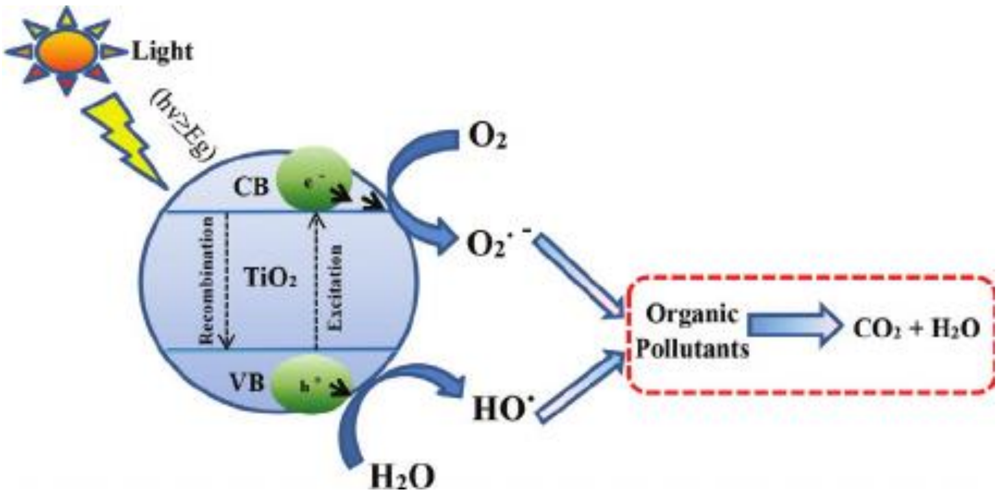
My reading has shown that the developed countries have already invested a lot of money into research, in order to improve production technologies so that they can maximise the impact of environmental protection. Scientists are searching for a solution in order to deal with the damage done in the past. The topic of my project involves advanced oxidation processes while focusing on the photocatalytic reaction.

In India (Beach in Mumbai, summer 2017)

For more than 45 years, photocatalysis has been given considerable attention, in connection with its potential use in environmental protection[1].

I want to find another means to use photcatalysis in a more efficient way and I am driven by the potential impact this could have on the fight to reduce river pollution.

Photocatalysis is a process in which irradiation induces a degradation of organic substances by means of hydroxyl radicals, which are the resultant product of the photocatalytic process. In order for this process to work, a photocatalyst is needed, triggering all the necessary processes[3,4].

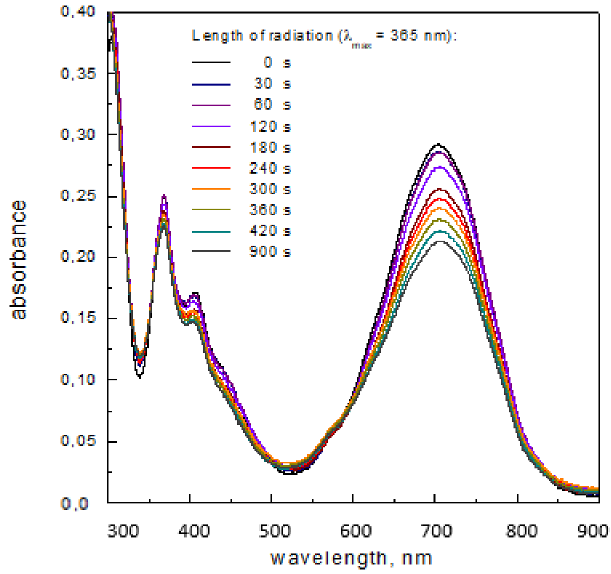


One of the most suitable materials used for photocatalytic processes in industrial and environmental applications is titanium dioxide TiO2. Titanium dioxide is relatively inexpensive, health-friendly and chemically stable. Its photocatalytic effects have a significant environmental benefit. Nevertheless, it has its limits of usability, so the chemical development is also focused on the search for new types of photocatalysts. The ideal photocatalyst should be able to degrade a wide variety of pollutants by solar radiation. The aim of my project was to familiarise myself with the theory of photocatalysis and to test the photocatalytic activity of titanium dioxide and zinc oxide on selected model pollutants. This demonstrated they are most effective in the UV region of the electromagnetic spectrum. I then further tested a currently used photocatalyst, graphitic carbon nitride form A, this showed improvement but was still dependent on UV radiation. This means the photocatalyst is not effective for large areas of rivers [2].

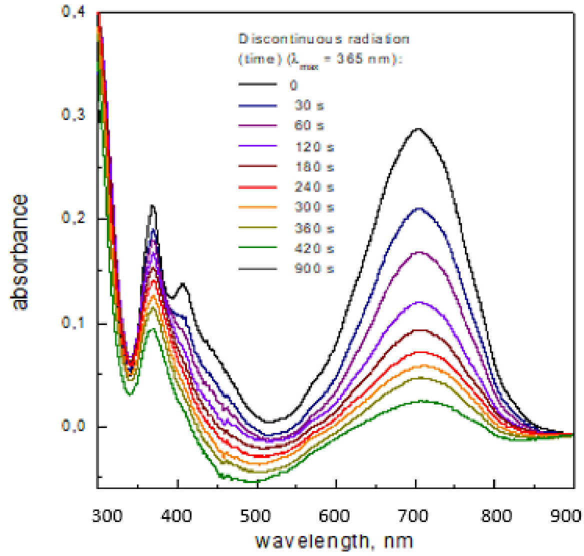
Learning of this, I decided to find a photocatalyst which would be able to produce radicals after absorbing wavelengths of visible light. By learning Quantum Chemistry methods and ZINDO/S AM1, I developed and adapted a new form of graphitic carbon nitride: g-C3N4 (form B). After cooperation with scientists from Greece who helped me produce g-C3N4 (form B) I continued my experimental work in the lab [4,5,6].

I investigated the efficiency of TiO_2, g-C_3N_4 g-C3N4(form A) and (form B) using UV/Vis spectrometry...

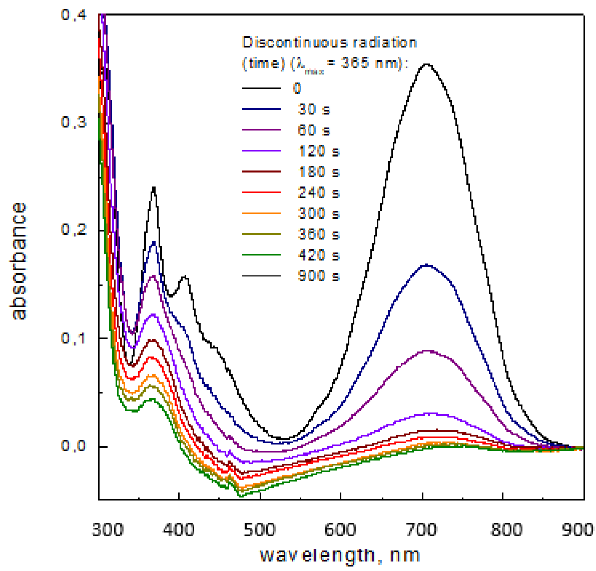
2.1 Photocatalyc degradation of DCIP and used irradiation equipment (UV/Vis spectrometer and KEVA with LED diodes)



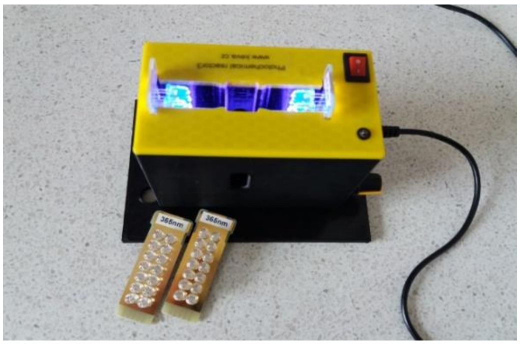
UV/Vis 1 **Changes in UV/Vis spectra of aqueous solution DCIP/TiO_2**



UV/Vis 2 **Changes in UV/Vis spectra of aqueous solution DCIP/g-C_3N_4 (form A)**



UV/Vis 3 **UV/Vis 1 Changes in UV/Vis spectra of aqueous solution DCIP/g-C3N4 (form B)**

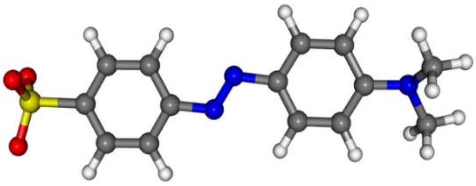
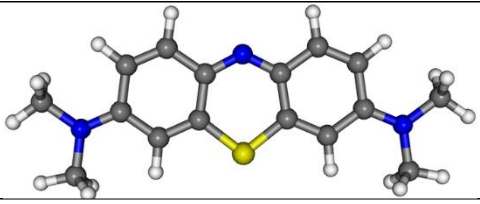
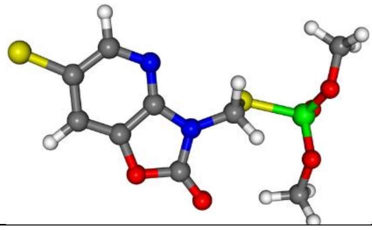
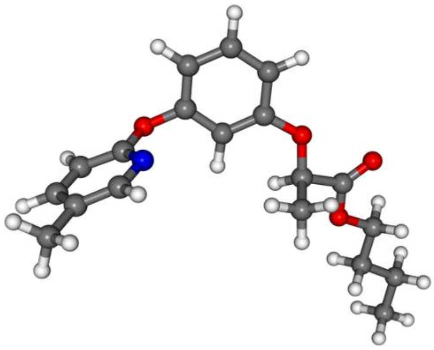


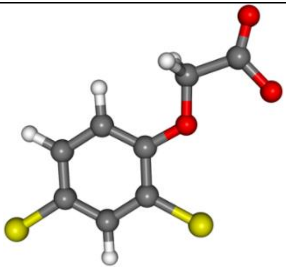
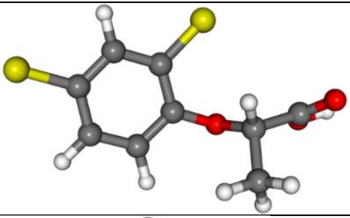
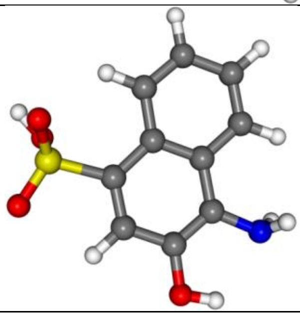
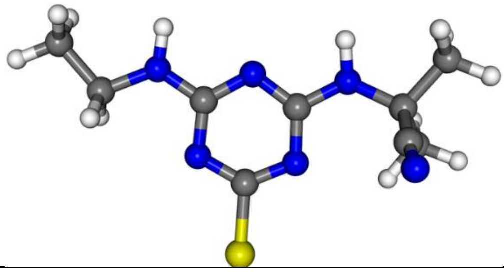
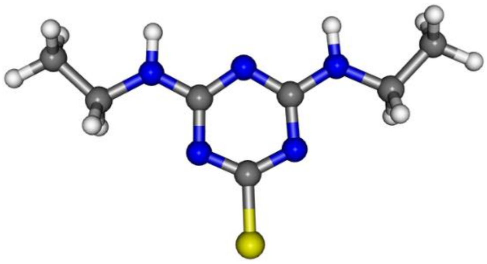
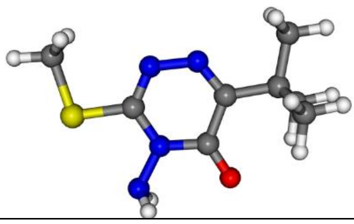
The results showed that graphitic carbon nitride has amazing properties including being an effective photocatalyst on model pollutants in the visible spectrum. I imagine sprinkling g-C3N4 (form B) into rivers and looking forward to a reduction in pollutants and cleaner waters.

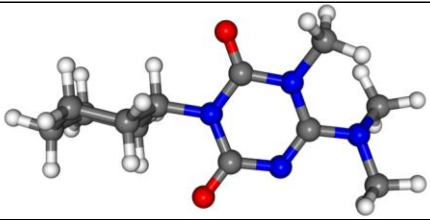
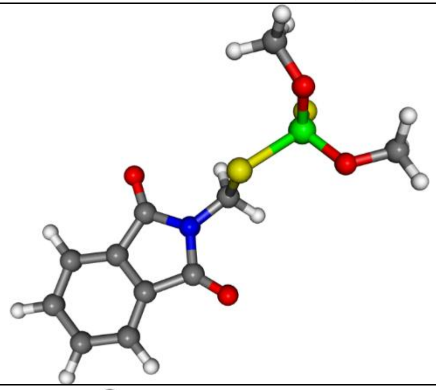
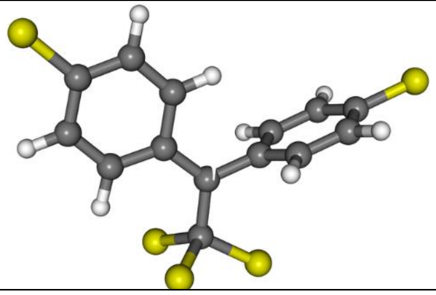
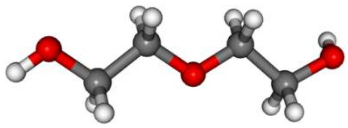
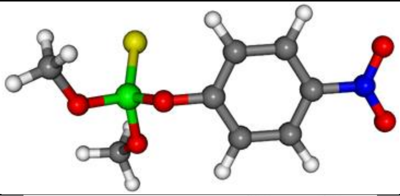
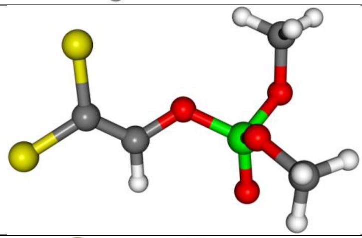
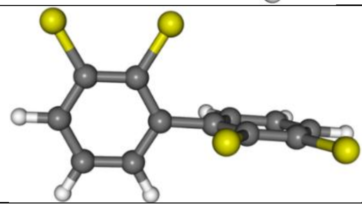
In order to achieve the objectives of the project I separated my process into two parts: theoretical and experimental. The theoretical part of the project was the assessment and selection of suitable model compounds for photocatalysis based on the elementary division of pollutants. The choice had to take into account the structural motifs of molecules used in the textile, agricultural and pollutant industries[4]. I had to use a wide variety of chemical databases and literature from chemistry journals to source the information. Similarly, I had to undertake a review of currently used and recently developed photocatalysts. Using quantum chemistry methods, I calculated the optimal geometry and electron structure of the photocatalyst, as well as the model compound to be studied experimentally. The experimental section of the project involved the study of the photocatalytic degradation of model compounds in the presence of selected photocatalysts by spectroscopy.

2.2 My selection of model compounds suitable for the study of photocatalytic degradation. Optimal geometry calculated by AM1. Boundary orbital values HOMO and LUMO in eV.

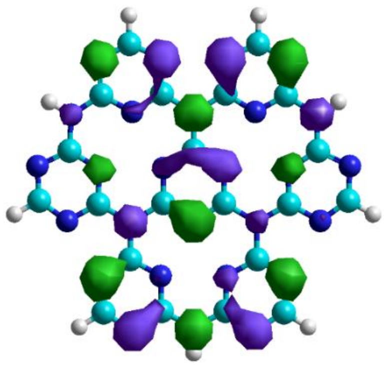
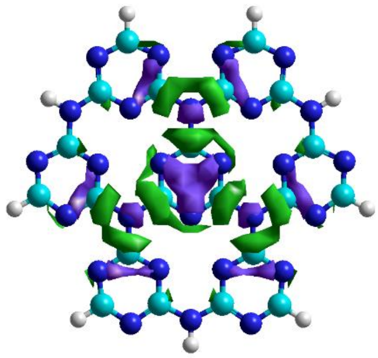
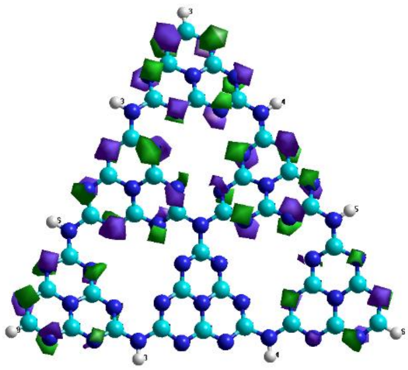
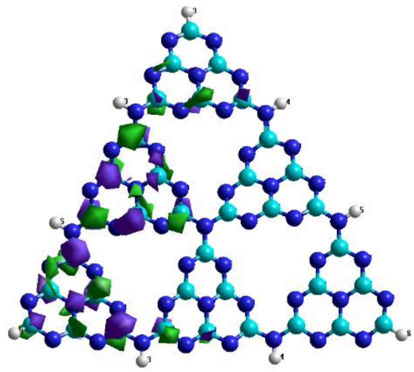
I completed visualization of the model compounds in chemistry software Molekel.

Compound	CAS number	Molekel	HOMO	LUMO
Methylene orange C2	**547-58-0**		-5.53 eV	3,07 (eV)
Methylene blue D1	**61-73-4**		-10,39 eV	-3,21 (eV)
Azamethiphos D3	**35575-96-3**		-9,21 (eV)	1,39 (eV)
Fluazifop-P- BUTYL H1	**79241-46-6**		-10,53 (eV)	-9,14 (eV)

Dichlorophenoxyacetic acid (2,4-D) H3	**94-75-7**		-9,24 (eV)	1,13 (eV)
2,4-Dichlorophenoxy propionic acid (2,4-DP) H4	**120-36-5**		-9,33 (eV)	1,68 (eV)
1-Amino- 2-naphthol-4-sulfonic acid H5	**116-63-2**		-8,38 (eV)	1,42 (eV)
Cyanazine H6	**21725-46-2**		-10,09 (eV)	1,57 (eV)
Simazine H7	**122-34-9**		-9,80 (eV)	1,78 (eV)
Metribuzin H8	**21087-64-9**		-9,27 (eV)	1,64 (eV)

Hexazinon H9	**51235-04-2**		-10,31 (eV)	1,55 (eV)
Fosmet H10	**732-11-6**		-9,42 (eV)	1,25 (eV)
Dichlorodiphenyl-trichlorethaneP1	**50-29-3**		-9,98 (eV)	1,42 (eV)
Diethylene glycol P3	**111-46-6**		-11,62 (eV)	2,00 (eV)
Parathion methyl P4	**298-00-0**		-9,87 (eV)	1,30 (eV)
Dichlorvos P5	**62-73-7**		-9,85 (eV)	1,57 (eV)
Polychlorinated biphenyls P2a	**1336-36-3**		-9,42 (eV)	1,60 (eV)

2.3 AM1 optimal geometry of DCIP and two forms of the g- C_3N_4 (A) and g- C_3N_4 (B) catalysts. Boundary molecular energy values are in eV.

	
HOMO -9.90 eV	**LUMO / –1.19 eV**
	
HOMO / –9.66 eV	LUMO / –2.45 eV

To start my project, I undertook further research into pollution; how it is categorised, the most significant sources of contamination, the effect on the environment and the extent of the problem. I knew I would have to learn the theory of advanced oxidation processes, including the Fenton reaction and photocatalysis. This was a challenging stage, so I was pleased to achieve a clearly written summary for my final report. I then evaluated the current state of photodegradation by researching through various citation databases, such as SCOPUS (www.scopus.com) and Web-of-Knowledge, available at FCHPT STU in Bratislava. The articles offered by both Elsevier and J Willey were equally accessible. In addition, published papers from other publishers were available from the websites of various research teams around the world. I had to significantly improve my scientific research skills before my work could benefit from this research so it took time to take the project forward from this theoretical research. I then had to learn how to use quantum chemical calculations which I performed using semi-empirical methods, using the ARGUS program (www.arguslab.com). Based on these theoretical calculations, I then predicted various molecular characteristics, such as the optimal structure, dipole moment, charge distribution, and the energy of boundary orbital. I calculated the optimal geometries and energies of boundary molecular orbits by the AM1 method and optical transitions by the ZINDO/S method. I then had to develop my ICT skills to present my work using the Molekel program (www.ugovaretto.github.io) to display the molecules, and the charts were drawn by Excel and Origin.
As I moved onto the experimental part of my project I approached the Institute of Chemistry in Bratislava. I asked if I could develop my theoretical research using their facilities and expertise. I

realized that I would need to invest further time to master the required techniques to a deeper level. When I began my experimental work, I used the following chemicals: titanium dioxide photocatalysts (TiO2; P25 Aeroxid, Evonik), zinc oxide (ZnO, nanoparticles, Sigma-Aldrich), graphitic carbon nitride (g-C3N4(Form A)) and graphitic carbon nitride (g-C3N4(Form B)) synthetized in the group of scientists, Institute of Demokritos, Athens (Greece). 2,6-dichloroindophenol sodium (DCIP, Sigma-Aldrich) and methylene blue (MB, 3,7-bis (dimethylamino)-phenazathionium chloride, Sigma-Aldrich) were used as model compounds for photodegradation. I used deionized water as the solvent.
The baseline photocatalyst concentrations were 1 mg mL-1 and model compounds 1.0 mmol L-1. I mixed suspensions of photocatalysts on the Tesla ultrasonic cleaner (in Piešťany) and the homogenizer (LabDancer, IKA). I measured UV/vis spectra on a UV/Vis/NIR UV3600 instrument (Shimadzu, USA) at 25 °C.
I measured individual spectra in a 1cm (0.4 inch) thick silicious cuvette with a volume of 3 mL. The reference solution was represented by the corresponding photocatalyst suspensions prepared by mixing 100 µL of a 1 mg mL-1 suspension and 2900 µL of water. All of my UV/VIS measurements were performed in the presence of molecular oxygen. The measurement of concentration dependence was based on the initial concentration of 100 µM and subsequently diluted in a ratio of 2/3 to the previous concentration. In photochemical UV/vis experiments, I prepared reaction systems by mixing 100 µL of a 1 mg mL-1 suspension, 2900 µL of water, and adding 30 µL of MB or 50 µL of DCIP. First, the spectrum of the given irradiated suspension was measured and then the sample irradiated for a defined period of time and the spectrum was measured. I irradiated the solutions with a KEVA irradiation device with monochromatic LED diodes (KEVA, Czech Republic) with λmax = 365 nm, λmax = 405 nm and λmax = 450 nm. The spectra were then processed in the ORIGIN (MicroCal) program.
I then determined a correct format for scientific reports and presented my work in detailed written form.

2.4 Values of wavelengths and oscillator forces calculated by the method of ZINDO/S for AM1 optimal geometry of g-C_3N_4 (form A).

g-C_3N_4(A)		
Optical transfer	**Wavelength in nm**	**Oscillator strength**
$S_0 \rightarrow S_1$	401	0,00
$S_0 \rightarrow S_2$	398	0,000858
$S_0 \rightarrow S_3$	397	0,000125
$S_0 \rightarrow S_4$	394	0,006
$S_0 \rightarrow S_5$	375	0,00034
$S_0 \rightarrow S_6$	374	0,000002
$S_0 \rightarrow S_7$	367	0,035
$S_0 \rightarrow S_8$	361,1	0,000001
$S_0 \rightarrow S_9$	361	0,000088
$S_0 \rightarrow S_{10}$	355	0,015

2.5 Values of wavelengths and oscillator forces calculated by the method of ZINDO/S for AM1 optimal geometry of g-C_3N_4 (form B).

g-C_3N_4(B)		
Optical transfer	**Wavelength in nm**	**Oscillator strength**
$S_0 \rightarrow S_1$	451	0,0025
$S_0 \rightarrow S_2$	449	0,014
$S_0 \rightarrow S_3$	447	0,011
$S_0 \rightarrow S_4$	445	0,000297
$S_0 \rightarrow S_5$	439	0,005
$S_0 \rightarrow S_6$	438	0,002
$S_0 \rightarrow S_7$	368	0,05
$S0 \rightarrow S_8$	361	0,063
$S_0 \rightarrow S_9$	351	0,194
$S_0 \rightarrow S_{10}$	350	0,078

3 Results

Based on my research work using citation databases, journal databases, and materials sourced from commercial chemical companies, I have determined a selection of molecules that could serve as model compounds for photodegradation. At the same time, I have given an overview of the molecular optimal geometry calculated by the semiempricic AM1 method. My calculations suggest that aromatic molecules, or their parts, are planar, with the attached substituents being able to produce different conformations with respect to spatial orientation. Higher Occupied Molecular Orbitals (HOMO) energies ranged from -5.53 eV for methylene orange to -11.62 eV for diethylene glycol. On the other hand, the energy values of the lowest unoccupied molecular orbital (LUMO) are within the range of -9,14 eV for Fluazifop-P-Butyl to -3,07 for methylene orange.
Based on the literary sources, I decided to study the photocatalyst g-C3N4 form A, which currently belongs to the newest types. The theoretical calculation suggested that the second form has a smaller difference in orbital energies, i.e. for HOMO it is -9.66 eV and for LUMO it is -2.45 eV. My calculations of optical transitions for the DCIP molecule indicated that for the wavelength of 393 nm, the optical transition from the base state to the third excited state would occur. The oscillator strength is very high (1.11) compared to other transitions. In the case of a photocatalyst, only g-C3N4 (B) shows enough intense oscillator force for the transfer between S0 → S2 with a wavelength of 449 nm. The second form will absorb significant light up within the UV region, i.e. for 367 nm. This suggests that the second form is less advantageous for photodegradation for less energy potent light. The theoretical data obtained are consistent with experimental wavelengths, i.e. 365 and 405 nm (form A) and 365 and 450

(form B).

4 The future and the use of newly designed photocatalysts

I think that this new modification could be used as the part of photoreactor set in the sewage plants and would me more effective in cleaning rivers.

The photocatalytic reactor for water treatment would be slurry type. The powdered catalyst (g-C_3N_4) is suspended in liquid.

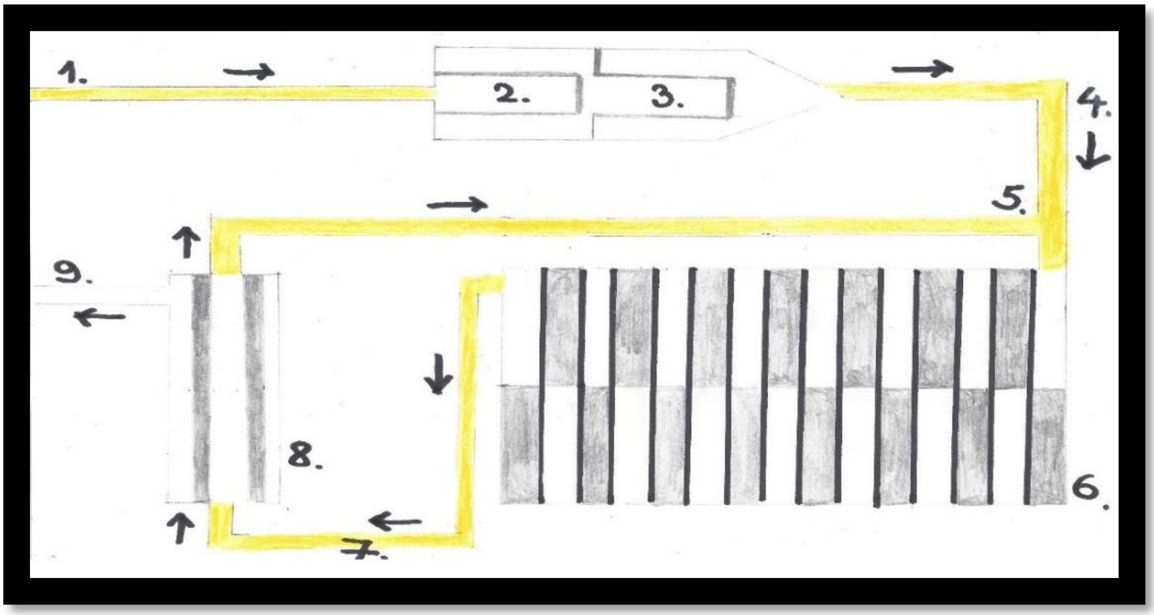
The main advantages of that:
- simple configuration
- high contact surface,

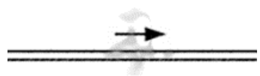
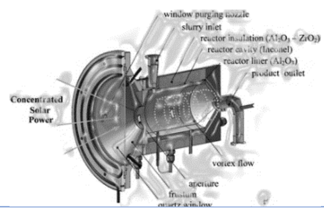
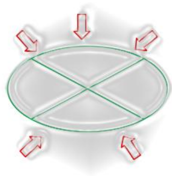
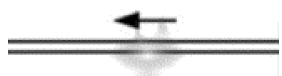
The immobilization of nanoscale photocatalyst can eliminate costly and impractical post-treatment recovery of spent photocatalysts for full-scale implementation. Substrate used for immobilization include glass, ceramic membranes, polymers, membrane cellulosic materials, optical fibers, and metallic supports, among others. These coated materials would be placed within the photocatalytic reactor, on the reactor walls, or even on the lamps, avoiding the separation and recovery stages. The immobilized photocatalysts must fulfil some requirements that depend on both the nanoscale semiconductor and the substrate:

(i) strong interaction between the semiconductor and the substrate
(ii) high chemical and physical stability of both,
(iii) high surface area for adsorption of the contaminant
(iv) the semiconductor must hold its photocatalytic efficiency after immobilization.

My general scheme of photocatalytic reactor

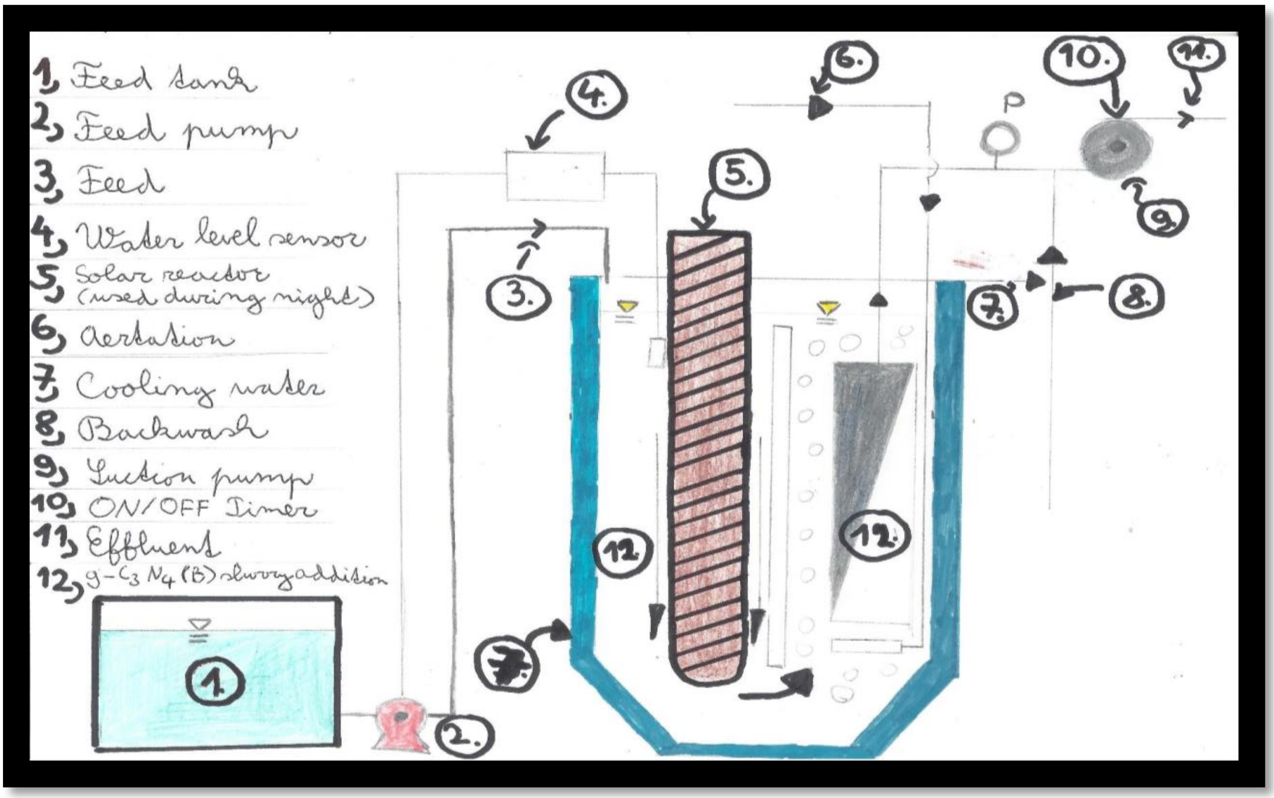
The photocatalytic reactor would be made of glass with large surface area.



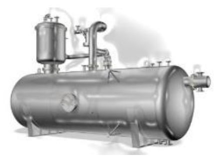
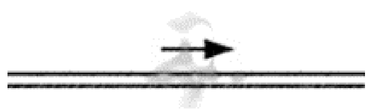
1)	**Raw water feed (polluted river)**	
2)	Bag filter	
3)	Cartridge filter	
4)	Influent sampling location	
5)	g-C_3N_4 (B) slurry addition	
6)	solar reactor (used during night)	
7)	Sampling location for g-C_3N_4 (B)	
8)	g-C_3N_4 recovery unit	
9)	Effluent sampling location	

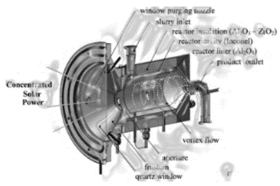
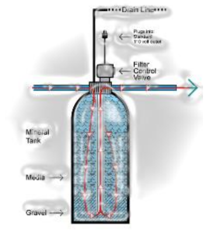
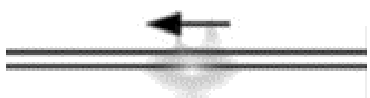
My scheme of membrane of the photocatalytic reactor which would be submerged

(which could be used as the part of sewage plants)



The advantage of using the photoreactor as the part of whole system is that the photocatalyst returns to the photoreactor while the concentration of the photocatalyst is maintained.

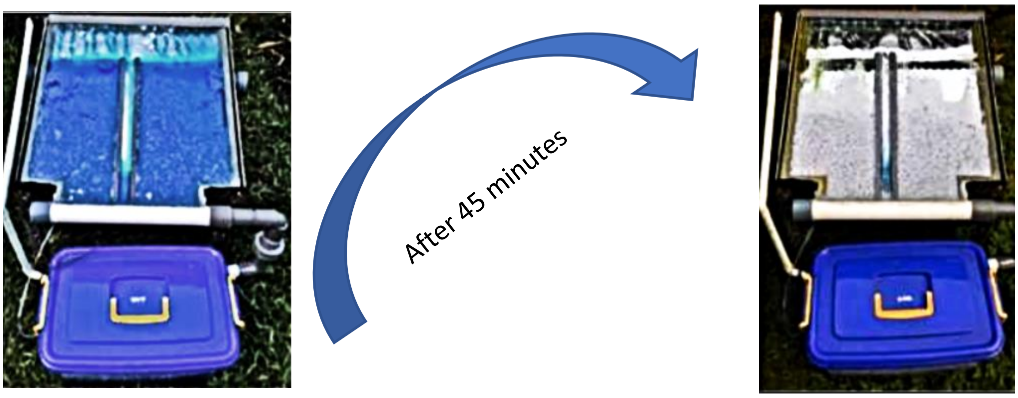
1)	Feed tank	
2)	Feed pump	
3)	Feed	

4)	Water level sensor	
5)	Solar reactor (used during night)	
6)	Aertation	
7)	Cooling water	
8)	Backwash	
9)	Suction pump	
10)	ON/OFF Timer	
11)	Effluent	
12)	g-C_3N_4 (B) slurry addition	

4.1 Simple experiment with homemade photoreactor and MB

I made a simple experiment to demonstrate the efficiency of photocatalyst and homemade water cleaning system with photoreactor submerged in water. (used pollutant -MB).

MB was completely eliminated after 45 minutes in dark condition after using solar photoreactor and slurry of g-C_3N_4 (B)



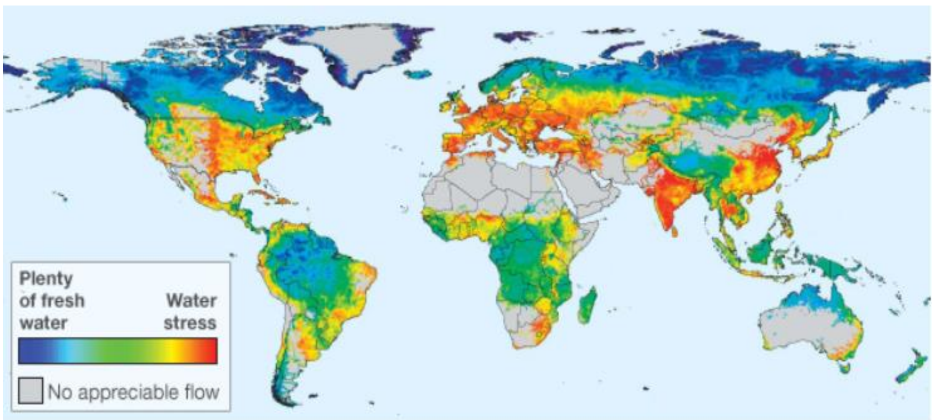
4.2 Comparison of the average cost and availability of the new photocatalyst in different countries around the world

We will need pure melamine for the production of g-C_3N_4. The prices are compared below. The melamine is of the same purity. The another expense would be energy required for the process of annealing.

Europe	(0.06 USD/kilogram)
Asia	**(1.44 USD/kilogram)**
Africa	**(0.04 USD/kilogram)**
America	**(0.06 USD/kilogram)**

4.3 The places where the primary help in cleaning rivers is needed

This is the map that show the billions at risk of water security. This map shows us that much of western Europe and North America appears to be under high stress. However, when the impact of the infrastructure that distributes and conserves water is added in the map the result is that most of the serious threat disappears from these regions. Africa, however, moves in the opposite direction.



> "A 2016 preliminary assessment of the water quality situation in Latin America, Africa and Asia, *A Snapshot of the World's Water Quality*, estimates that sever pathogenic pollution affects around one third of all rivers, severe organic pollution around one seventh of all rivers, and severe and moderate salinity pollution around one tenth of all rivers in these regions."

For me, what is even more valuable is showing the world that we can use quantum chemistry software and calculations in terms of photocatalysis. I really want to show the world that this is the way to inspire students. If we want to clean polluted rivers we have to focus on photocatalysis and study physical chemistry.

5 Discussion

Following my set objectives, I found a selection of suitable model substances which can be used in laboratory photodegradation testing and I completed this testing with success. Boundary orbital energy values are within a range similar to that of the investigated photocatalyst. The compounds are also available as commercial compounds. The photodegradation of the DCIP molecule (2,6-dichloroindophenol) with g-C3N4 (graphitic carbon nitride) by photocatalyst has been experimentally studied. The results indicated that the photocatalyst can work for the wavelength range from 365 to 405 nm (form A) and 365-451 (form B). The catalyst can successfully generate hydroxyl radicals. I performed theoretical calculations of optimal geometries of selected molecules and the values of boundary molecular orbital energies were compared to each other. In addition, computed wavelengths of the optical transitions of the researched molecule DCIP and g-C3N4 were compared. Research of this class of catalytic converters cannot be considered as completed. It will be necessary to propose a modification of the boron and nitrogen photocatalyst so that the optical transitions are moved further into the visible region of the spectrum. Based on my work, the catalyst I have identified and tested could be developed on a commercial scale to reduce river pollutants. Nowadays, photocatalysis is also used directly in sewage plants in the form of superstructures using photocatalysts therefore g-C_3N_4 (form B) would be the best candidate.

So I am hoping that this competition will open doors to give this research to companies and individuals who could develop the photocatalyst in this way.

In India (village Tirunilai, near Chennai, summer 2018)

6 Conclusions

I decided to find the photocatalyst which would be able to produce radicals after absorbing wavelengths of visible light. I used quantum chemistry software and finally found graphitic carbon nitride : g-C_3N_4 (form B). After cooperation with scientists from Greece who helped me synthetize g-C_3N_4 (form B) I continued my experimental work and confirmed the efficiency of this newly designed phtocatalyst.

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