4-2. IROAST Seminars

No. (invitation Program No.)	Title / Date	IROAST Speaker / Organizer
4-2-1 (3-1-3)	The 84th IROAST Seminar - Computer vision and its applications in the New Zealand blue economy	**Patrice DELMAS** The University of Auckland
	December 7, 2022	**Toshifumi MUKUNOKI** FAST
4-2-2 (3-1-4)	The 85th IROAST Seminar - Operando investigations of gas sensing with semiconducting metal oxides	**Nicolae BARSAN** University of Tubingen
	October 13, 2022	**Tetsuya KIDA** FAST
4-2-3 (3-1-5)	The 86th IROAST Seminar - A-Z of Biorefinery: A Promising Approach Towards Sustainable Bio-Circular-Green Economy Development	**Suttichai ASSABUMRUNGRAT** Chulalongkorn University
	October 28, 2022	**Tetsuya KIDA** FAST
4-2-4 (3-1-6)	The 87th IROAST Seminar - Workshop on the fundamentals of grain boundary phenomena	**Pavel LEJČEK** Institute of Physics, Academy of Sciences of Czech Republic
	November 1, 2022	**Sadahiro TSUREKAWA** FAST
4-2-5 (3-1-7)	The 88th IROAST Seminar - Historical-ecology of the COVID pandemic- The 89th IROAST Seminar - The international impact of Japanese nutritional science and policy (1920-1945)-	**Josep Lluís BARONA-VILAR** University of Valencia
	88th: November 29, 2022 89th: December 2, 2022	**Makoto TAKAFUJI** FAST
4-2-6 (3-1-8)	The 90th IROAST Seminar - The 3D Modular Building Connections (3DMBC) project	**Konstantinos Daniel TSAVDARIDIS** City, University of London
	February 2, 2023	**Gaochuang CAI** IROAST
4-2-7 (3-1-9)	The 91st IROAST Seminar -From Metal-Metal Multiple Bonds to Helical Metal Strings	**Shie-Ming PENG** National Taiwan University
	February 14, 2023	**Shinya HAYAMI** FAST

4-2-8 (3-1-10)	The 92nd IROAST Seminar Subcritical water for waste treatment and biomass valorisation	**Olivier BOUTIN** Aix-Marseille University
	February 17, 2023	**Mitsuru SASAKI** IINa
4-2-9 (3-1-11)	The 93rd IROAST Seminar Metal oxide nanostructures as building blocks for energy and environmental application	**Dario ZAPPA** The University of Brescia
	March 1, 2023	**Tetsuya KIDA** FAST

FAST: Faculty of Advanced Science and Technology

IINa: Institute of Industrial Nanomaterial

IROAST Seminar & Research Activity Report by IROAST Visiting (Associate) Professor Invitation

No.3-1-3 (Invitation Program) No.4-2-1 (Seminar)	Name	Patrice DELMAS	Title	Associate Professor
	Affiliation	The University of Auckland, Australia		
Host Faculty	Name	Toshifumi MUKUNOKI	Title	Professor
	Affiliation	Faculty of Advanced Science and Technology（FAST）		
Seminar Title	84th IROAST Seminar- Computer vision and its applications in the New Zealand blue economy			
Venue	100th Anniversary Hall, Kumamoto University			
Time & Date	15:25-16:05, December 7, 2022			
Speaker's Name/ Title/Affiliation	Patrice DELMAS, Associate Professor, Department of Computer Science, The University of Auckland, NZ			
Number of Participants	Total: 25 in person and 36 online (Int'l participants: 24) Invitees: 18 (Int'l participants: 9)			
Duration of Visit	From December 2, 2022- December 8, 2022			

The 9th international workshop on X-Earth called as IWX2022 was held on Dec.6-7th. This workshop has been continued since 2010 and the researchers using X-ray CT have gathered at Kumamoto University. Even if the research background is different from each other, they can discuss and share the knowledge of "Image analysis". Dr. Delmas is the specialist of Computer vision so he has been invited since 2016 to IWX.

Dr. Delmas gave his lecture at the IROAST session on Dec.7. He has a large UAV which can load three different types of cameras and scan on the surface of estuary in Auckland. He has contributed to marine science by taking photo from UAV and analyze the surface condition using hyperspectral camera. He gave us the impact of the effectiveness using computer vision to the audience.

Advanced Concepts for Intelligent Vision systems (ACIVS) 2023 will be held on Kumamoto (KKR hotel) from Aug. 21 to 24th. Dr. Delmas is a keyperson of this conference and Dr. Mukunoki and Dr. Otani have been invited as scientific committee members already. During this conference, Dr. Delmas and Dr. Mukunoki will organize the IROAST session and collect some paper. Excellent paper will be upgraded to the journal paper.

Opening Remarks
Professor Hisao Ogawa,
President of Kumamoto University

University Introduction
Professor Toshifumi Mukunoki,
Head of X-Earth Center

Associate Professor, Patrice Delmas, IROAST Visiting Professor, The University of Auckland

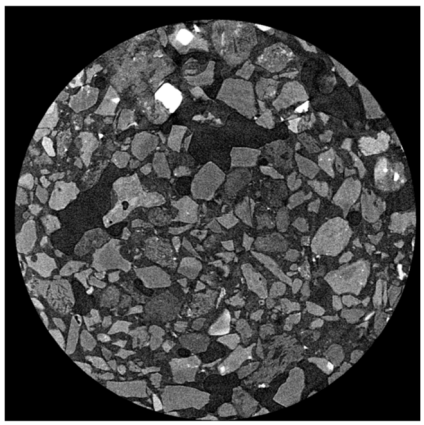
Professor Jun Otani,
Vice President of Kumamoto University

At venue

-Activities report with visiting (associate) professor-

The purpose of his visiting was not to perform research concretely but give his lecture so there is no achievement in this visiting. Just. Dr. Delmas discussed future with Dr. Mukunoki clearly.

Dr. Delmas and Dr. Mukunoki will start new research topic for “Blue carbon” in Carbon Neutral Project. Already, Dr. Mukunoki take sample from the estuary and scan the soil to visualize the pore structure. On the other hand, Dr. Delmas has scan the estuary by the hyperspectral camera in Auckland and he discover the potential of Blue carbon project



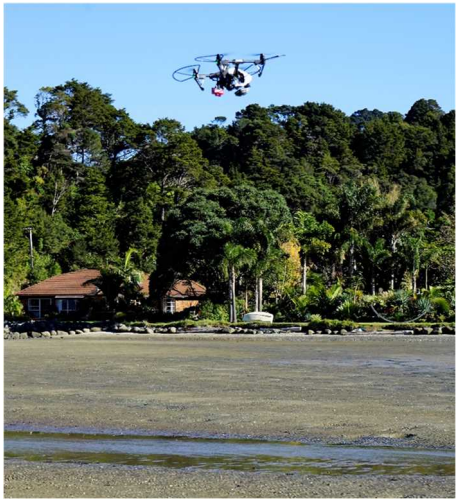


Fig. 1 Nano-focused CT image of mud soil.
Photo. UAV during the scanning mud soil at Auckland

IROAST Seminar & Research Activity Report by IROAST Visiting (Associate) Professor Invitation

No.3-1-4 (Invitation Program) No.4-2-2 (Seminar)	Name	Nicolae BARSAN	Title	Senior Researcher
	Affiliation	The Institute of Physical and Theoretical Chemistry, University of Tubingen, Germany		
Host Faculty	Name	Tetsuya KIDA	Title	Professor
	Affiliation	Faculty of Advanced Science and Technology (FAST)		
Seminar Title	The 85th IROAST Seminar -Operando investigations of gas sensing with semiconducting metal oxides			
Style	Kurokami South W4 (Faculty of Engineering Research Bldg. II) 2F Conference Room			
Time & Date	16:00-17:00, October 13, 2022			
Speaker's Name/ Title/Affiliation	Nicolae BARSAN Senior Researcher, The Institute of Physical and Theoretical Chemistry, University of Tubingen, Germany			
Number of Participants	Total: 34 (Int'l participants: 8) Invitees: 5 (Int'l participants: 2)			
Duration of Visit	From October 13, 2022- October 19, 2022			

In the seminar, Dr. Barsan spoke about gas sensing with semiconductor metal oxide-based devices, explaining that the operando approach has proven to be very effective in understanding gas sensing mechanisms. The talk included examples of the use of two of the most successful methods including Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS) and Kelvin probe work function change measurements. In both cases, the DC resistance of the sensor was measured simultaneously. The analysis covered the effect of water vapor on the conduction and reception functions of SnO_2-based sensors and the surface reaction of WO_3-based gas sensors when exposed to ethanol and acetone.

This seminar and lecture broadened the perspectives of the participating researchers and students on the science and technology of gas sensing using semiconductor materials. Before and after the seminar, the possibility of future collaborative research and international joint publications were also discussed. Plans to exchange students were also agreed upon. The host professor plans to send an assistant professor, one post-doctoral fellow, and two graduate students to Tubingen for joint research.

Dr. Nicolae Barsan,

THE 85TH
IROAST SEMINAR

October 13, 2022
16:00-17:00

Lecture Title

Operando investigations of gas sensing with semiconducting metal oxides

@ Kurokami South W4
(Faculty of Eng. Research Bldg. II)
2F Conference Room

Lecturer

Dr. Nicolae Barsan

The Institute of Physical and Theoretical Chemistry, University of Tubingen, Germany

Organizer: Prof. Tetsuya Kida
Faculty of Advanced Science and Technology, KU

Contact: IROAST Phone: 096-342-3362 E-mail: szk-kiko@jimu.kumamoto-u.ac.jp Web: http://iroast.kumamoto-u.ac.jp/

IROAST Seminar & Research Activity Report by IROAST Visiting (Associate) Professor Invitation

<table>
<tr><td rowspan="2">No.3-1-5
(Invitation Program)
No.4-2-3
(Seminar)</td><td>Name</td><td>Suttichai ASSABUMRUNGRAT</td><td>Title</td><td>Professor</td></tr>
<tr><td>Affiliation</td><td colspan="3">Chulalongkorn University, Thailand</td></tr>
<tr><td rowspan="2">Host Faculty</td><td>Name</td><td>Tetsuya KIDA</td><td>Title</td><td>Professor</td></tr>
<tr><td>Affiliation</td><td colspan="3">Faculty of Advanced Science and Technology (FAST)</td></tr>
<tr><td>Seminar Title</td><td colspan="4">86th IROAST Seminar- A-Z of Biorefinery: A Promising Approach Towards Sustainable Bio-Circular-Green Economy Development</td></tr>
<tr><td>Style</td><td colspan="4">Hybrid (via Zoom and on-site)
Kurokami North E6: College of Cross-Cultural and Multidisciplinary Studies (Center for International Education) Room 1A</td></tr>
<tr><td>Time & Date</td><td colspan="4">13:00-14:30, October 28, 2022</td></tr>
<tr><td>Speaker’s Name/ Title/Affiliation</td><td colspan="4">Suttichai ASSABUMNGRAT, Professor,
Center of Excellence in Catalysis and Catalytic Reaction Engineering, Department of Chemical Engineering, Faculty of Engineering, Biorefinery Cluster,
Bio-Circular-Green economy Technology & Engineering Center, Department of Chemical Engineering, Faculty of Engineering,
Chulalongkorn University, Thailand</td></tr>
<tr><td>Number of Participants</td><td colspan="4">Total: 70 (Int’l participants: 46)
Invitees: 1 (Int’l participants: 1)</td></tr>
<tr><td>Duration of Visit</td><td colspan="4">From October 24,2022-October 28, 2022</td></tr>
</table>

The seminar given by Prof. Suttichai Assabumrungrat focused on the concept of biorefinery to support the Bio-Circular-Green Economy development and the United Nation’s Sustainable Development Goals (SDGs). Some key important topics were addressed including overviews of biorefinery, biomass and biobased products, conversion of biomass to high-value products, downstream recovery and separation, process creation, design and analysis, and case studies.

This seminar has broadened the knowledge of participating researchers and students (both online and on-site) on many aspects of “biorefinery”. Activities other than the seminar were as follows:

1. Discussion on the revision of our joint research paper titled “In-situ Transesterification of Microalgae using Carbon-Based Catalyst under Pulsed Microwave Irradiation”, which has been recently accepted for publication in a reputable journal in this field – “Biomass and Bioenergy”.
2. Updates on our on-going e-ASIA Project on Algal Biomass (SICORP-funded research project), and follow-up on future joint research applications (JSPS Bilateral Joint Research Project/SATREPS).
3. Strengthening future collaboration on research and academic exchanges was also discussed. For this purpose, 2 professors, 1 assistant professor, 1 post-doctoral fellow and 10 students (partly funded by JASSO) will go to Thailand for academic, cultural and research exchanges this academic year 2022.

Opening: Prof. Armando T. Quitain

Group Photo

Professor Suttichai Assabumrungrat

IROAST Seminar & Research Activity Report by IROAST Visiting (Associate) Professor Invitation

<table>
<tr><td rowspan="2">No.3-1-6
(Invitation Program)
No.4-2-4
(Seminar)</td><td>Name</td><td>Pavel LEJČEK</td><td>Title</td><td>Professor</td></tr>
<tr><td>Affiliation</td><td colspan="3">Institute of Physics, Academy of Sciences of Czech Republic</td></tr>
<tr><td rowspan="2">Host Faculty</td><td>Name</td><td>Sadahiro TSUREKAWA</td><td>Title</td><td>Professor</td></tr>
<tr><td>Affiliation</td><td colspan="3">Faculty of Advanced Science and Technology (FAST)</td></tr>
<tr><td>Seminar Title</td><td colspan="4">The 87th IROAST Seminar ~Workshop on the fundamentals of grain boundary phenomena~</td></tr>
<tr><td>Style</td><td colspan="4">Hybrid via Zoom and on site; Kurokami South C8 Room222</td></tr>
<tr><td>Time & Date</td><td colspan="4">13:30-16:30, November 1, 2022</td></tr>
<tr><td>Speaker’s Name/
Title/Affiliation</td><td colspan="4">Pavel Lejček, Professor, IROAST Visiting Professor
Institute of Physics, Academy of Sciences of Czech Republic
Takahito Ohmura, Dr., Vice President of Research Center for Structural Materials (RCSM)
National Institute for Materials Science (NIMS)
Yukio Sato, Associate Professor,
Department of Materials, Kyushu University
Dmitri, A. Molodov, Professor, IROAST Distinguished Professor,
RWTH Aachen University, Germany</td></tr>
<tr><td>Number of Participants</td><td colspan="4">Total: 50 (Int’l participants: 12)
Invitees: 4 (Int’l participants: 2)</td></tr>
<tr><td>Duration of Visit</td><td colspan="4">From October 30, 2022-November 11, 2022</td></tr>
</table>

Report

During my stay at Kumamoto University, I participated at the above-mentioned meeting organized by prof. Sadahiro Tsurekawa under the auspices of IROAST and other organization. At this workshop I presented the results of my very recent research concerning the role of entropy in grain boundary segregation, mainly for the cases in which the entropy plays either the dominant role or even when it completely controls (drives) the segregation of the solutes. On the other hand, I became familiar with the recent results obtained at another laboratories of Kyushu University, NIMS and RWTH in Aachen/Germany.

According to my meaning, the seminar brought (according to my feeling) two important items. First, the participation of the students in the auditorium enabled them to become familiar with the top research at different laboratories. Based on our contributions and discussion, we arranged a plan of a joint collaboration in future involving the student exchange, mainly a stay of a Japanese student at our laboratory in Prague next year (if she will be selected for a trip to Europe). Second, the discussion with participants of the resulted in new ideas and we started a collaboration in the field of the entropy-driven grain boundary segregation which is a newly suggested phenomenon which needs urgently an experimental proof. We suppose that obtained experimental results supporting this suggestion would represent top results which will be competitive for publication in top scientific journals and bring a new understanding of the topic of grain boundary segregation.

Activities report with visiting (associate) professor

Besides the above-mentioned workshop, I got the possibility to discuss actual topics of diploma theses with students in the laboratory of prof. Tsurekawa. Many of these topics are very close to my interests and we could discuss a lot with the students. It is only pity that the students have some troubles in discussing in English. Nevertheless, we found a joint topic – study of the properties of so-called high-entropy alloys – which has been recently started at our laboratories. In this respect we did prepare samples for joint experiments and expect further close cooperation of our laboratories. This cooperation will be very welcome as we can share materials and use complementary techniques for investigation. Because my stay at the Kumamoto University was rather short (2 weeks), no joint experiments were performed during this time. In any case, I am very enthusiastic by the intensified cooperation and believe in its success in near future.

Opening; Prof. Sadahiro Tsurekawa

Prof. Pavel Lejček

Dr. Takahito Ohmura

Assoc. Prof. Yukio Sato

Prof. Dmitri, A. Molodov

Group Photo

THE 87TH

IROAST SEMINAR

WORKSHOP ON THE FUNDAMENTALS OF GRAIN BOUNDARY PHENOMENA

NOVEMBER 1 (TUE), 2022, 13:30-16:30

KUROKAMI SOUTH C8 ROOM222

(FACULTY OF ENGINEERING BLDG. 2)

PROGRAM

13:30 Opening Address

13:35- 14:20 Entropy Effect in Solute Segregation at Grain Boundaries
Professor Pavel Lejček, IROAST Visiting Professor,
Institute of Physics, Academy of Sciences of Czech Republic,
Czech Republic

14:20- 14:55 Microstructural and Nano-mechanical Characterization of Dislocation-Grain Boundary Interaction
Dr. Takahito Ohmura,
Vice President of Research Center for Structural Materials(RCSM)
National Institute for Materials Science (NIMS), Japan

14:55- 15:10 Break

15:10- 15:45 Grain boundary structure and electrical transport in ZnO bicrystals
Associate Professor Yukio Sato,
Department of Materials, Kyushu University, Japan

15:45 – 16:30 On shear-coupled grain boundary migration:
Model experiments on Al and Cu bicrystals
Professor Dmitri A. Molodov, IROAST Distinguished Professor,
RWTH Aachen University, Germany

16:30 Closing Address

Organizer: Sadahiro Tsurekawa, Fast, KU
turekawa@kumamoto-u.ac.jp
Simultaneous delivery via Zoom. Please contact Organizer for Zoom info

Contact: IROAST Phone: 096-342-3362 E-mail: szk-kiko@jimu.kumamoto-u.ac.jp Web: http://iroast.kumamoto-u.ac.jp/

IROAST Seminar & Research Activity Report by IROAST Visiting (Associate) Professor Invitation

<table>
<tr><td rowspan="2">No.3-1-7
(Invitation Program)
No.4-2-5
(Seminar)</td><td>Name</td><td>Josep Lluís BARONA-VILAR</td><td>Title</td><td>Professor</td></tr>
<tr><td>Affiliation</td><td colspan="3">University of Valencia, Spain</td></tr>
<tr><td rowspan="2">Host Faculty</td><td>Name</td><td>Makoto TAKAFUJI</td><td>Title</td><td>Professor</td></tr>
<tr><td>Affiliation</td><td colspan="3">Faculty of Advanced Science and Technology (FAST)</td></tr>
<tr><td>Seminar Title</td><td colspan="4">88th IROAST Seminar
- Historical-ecology of the COVID pandemic-
89th IROAST Seminar
- The international impact of Japanese nutritional science and policy (1920-1945)-</td></tr>
<tr><td>Venue</td><td colspan="4">203 Lecture room, Academic Commons Kurokami Bldg. 1</td></tr>
<tr><td>Time & Date</td><td colspan="4">15:00-16:00, November 29, 2022
11:00-12:00, December 2, 2022</td></tr>
<tr><td>Speaker’s Name/
Title/Affiliation</td><td colspan="4">Josep Lluís BARONA-VILAR, Professor,
University of Valencia, Spain</td></tr>
<tr><td>Number of
Participants</td><td colspan="4">Total: 41 (Int’l participants: 14)
Invitees: 1 (Int’l participants: 1)</td></tr>
<tr><td>Duration of Visit</td><td colspan="4">November 25, 2022- December 5, 2022</td></tr>
</table>

Prof Josep BARONA spoke on 'Historical-ecology of the COVID pandemic' and 'The international impact of Japanese nutritional science and policy (1920-1945)'. The first lecture was on the 'Historical-ecology of the COVID pandemic'.
In his first lecture, the professor gave a historical perspective on the plagues that have affected mankind since ancient times. He discussed the environmental, biological and social factors involved in historical pandemics in relation to time, living conditions, medicine and healthcare systems, and proposed the use of historical experience in analyzing and understanding current scientific, medical and technological issues.
In the second lecture, the professor introduced the Imperial Government Institute of Nutrition (IGIN, 1920), founded by Dr Masasuke Saiki in 1920, during a period of crisis characterized by war, famine, economic recession and global instability in the first half of the twentieth century. The international leadership and nutritional ideas of Dr Masuo Saiki, the important scientific and political role of IGIN, and the global network of scientific and diplomatic relations were presented.

1. Seminar Outcomes and Future Plan (e.g. about contribution to the development of young researchers and the initiation of international collaborative research aiming for the publication of international collaborative papers, etc.)

So far, members of Kumamoto University have collaborated with a research group at the University of Valencia on the chiroptic properties of supramolecular assemblies, with good results. We discussed ways to extend these results and promote new collaborations. We also discussed future research exchanges and the exchange of young researchers, including postgraduate students.

88th seminar

Opening talk by Prof. Takafuji

Professor Barona

At venue

89th seminar

Opening talk by Prof. Takafuji

Professor Barona

At venue

Group photo

2.Research achievements during his/her stay in Kumamoto University.
Prof. Josep BARONA has many discussions on research with young researchers during his stay at Kumamoto University. Multilateral discussions on research with visiting Lithuanian, Bangladeshi and Kyrgyz professors and researchers were also held during his stay.

3. Prospect for further research collaboration.
New joint research project was proposed and discussions were to continue towards obtaining research funding between the two organizations.

IROAST Seminar & Research Activity Report by IROAST Visiting (Associate) Professor Invitation

<table>
<tr><td rowspan="2">No. 3-1-8
(Invitation Program)
No. 4-2-6
(Seminar)</td><td>Name</td><td colspan="2">Konstantinos Daniel TSAVDARIDIS</td><td>Title</td><td>Professor</td></tr>
<tr><td>Affiliation</td><td colspan="4">City, University of London, UK</td></tr>
<tr><td rowspan="2">Host Faculty</td><td colspan="2">Name</td><td>Gaochuang CAI</td><td>Title</td><td>Associate Professor</td></tr>
<tr><td colspan="2">Affiliation</td><td colspan="3">IROAST</td></tr>
<tr><td>Seminar Title</td><td colspan="5">90th IROAST Seminar
The 3D Modular Building Connections(3DMBC) project</td></tr>
<tr><td>Venue</td><td colspan="5">Kurokami South C4 (Academic Commons Kurokami Bldg. 2) 2F Room204</td></tr>
<tr><td>Time & Date</td><td colspan="5">10:50-12:10, February 2, 2023</td></tr>
<tr><td>Speaker’s Name/
Title/Affiliation</td><td colspan="5">Konstantinos Daniel Tsavdaridis, Professor,
City, University of London, UK</td></tr>
<tr><td>Number of
Participants</td><td colspan="5">Total: 17 (Int’l participants: 9)
Invitees: 1 (Int’l participants: 1)</td></tr>
<tr><td>Duration of Visit</td><td colspan="5">January 29, 2023-February 3, 2023</td></tr>
</table>

-Seminar report -

1. Seminar Overview

The purpose of this seminar is to understand Professor Tsavdaridis's research on modular housing, especially the safety performance and countermeasures of the joints in the buildings, and based on this, to deeply discuss the research progress of housing and the possibility of implementation in Japan, as well as two research groups future research direction.

2. Seminar Outcomes and Future Plan (e.g. about contribution to the development of young researchers and the initiation of international collaborative research aiming for the publication of international collaborative papers, etc.)

-Seminar Outcomes

Based on this workshop, we will develop a new way of cooperation, including joint experimental analysis, remote mentoring of young PhDs and researchers, and at least one Ph.D. visit per year.

-Application of funding supports

JSPS-visiting researcher program

JST-SATREPS project

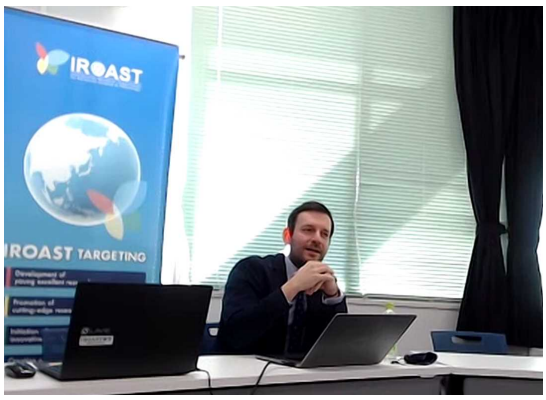
Kajima Foundation -Support Program for International Joint Research Activities (https://www.kajima-f.or.jp/en/)

- Publication of international collaborative papers

(1) **G. Cai***, Y. Wen, T. Fujinaga, **K. D. Tsavdaridis**, A. Si Larbi. Cyclic behavior and FE analysis of RCFT columns under simulated seismic loads, Structures (IF: 4.010), will be submitted by May 2023

(2) **G. Cai***, Y. Wen, T. Fujinaga, **K.D. Tsavdaridis**, A. Si Larbi. Cyclic behavior and FE analysis of RCFT columns under simulated seismic loads, Journal of Building Engineering (IF: 6.4), will be submitted by July 2023

Two papers are under perparation.



Prof. Konstantinos

Q&A, Discussion

At venue

Group photo

-Activities report with visiting (associate) professor-
-Host a symposium at Kumamoto University with Dr. Cai.
We hosted an international symposium during his stay at Kumamoto. The details are available on the IROAST website.

-Discussion on collaboration, including publication, and funding application.
We have discussed the details of the main collaboration topics, collaboration methods, etc.

-Offering an IROAST seminar
Professor TSAVDARIDIS offered a lecture entitled "The 3D Modular Building Connections (3DMBC) project and discussed it with the students.

-Visiting the structural lab at Kumamoto University for discussing the future research plan.
Professor TSAVDARIDIS visited the research lab. with another visitor with Dr. Cai for discussing the possibility of new research topics in the future.

3. Research achievements during his/her stay in Kumamoto University.

-Publication
Q. Su, G. Cai*, M. Hani, A. Si Larbi, **K. D. Tsavdaridis**. (2023) Damage control of the masonry infills in RC frames under cyclic loads: A full-scale test study and numerical analyses, Bulletin of Earthquake Engineering, 21, 1017–1045. (IF*4.556, Q1)

-Research exchange
A Ph.D. student will visit CITY next year

4. Prospect for further research collaboration.

-Funding application
Prepare a proposal for the following programs,
JST-SATREPS project

-Publication
More than 2 papers are under preparation with the professor

-Visiting exchange
Dr. Cai will visit the professor's university for having lectures, test collaboration, and seminar

IROAST Seminar & Research Activity Report by IROAST Visiting (Associate) Professor Invitation

No. 3-1-9 (Invitation Program) No. 4-2-7 (Seminar)	Name	Shie-Ming PENG	Title	Professor
	Affiliation	National Taiwan University, Taiwan		
Host Faculty	Name	Shinya HAYAMI	Title	Professor
	Affiliation	Faculty of Advanced Science and Technology（FAST）		
Seminar Title	91st IROAST Seminar From Metal-Metal Multiple Bonds to Helical Metal Strings			
Style	Online: Zoom Venue: Kurokami South E1 (Faculty of Science Bldg. 1 & 2) 2F C226			
Time & Date	14:30-16:00, February 14, 2023			
Speaker's Name/ Title/Affiliation	Shie-Ming Peng, Professor, IROAST Visiting Professor National Taiwan University, Taiwan			
Number of Participants	Total: 35 (Int'l participants: 7) Invitees: 1 (Int'l participants: 1)			
Duration of Visit	From February 10, 2023- March 11, 2023			

1. Seminar Overview
   In this seminar, the invited speaker Shie-Ming Peng gave a lecture about the recent advance in coordination chemistry, especially, the metal-metal multiple bonds to form helical metal strings. The metal-metal bonding complexes have fundamental features such as structures, spin, and electrical conductivity. Furthermore, the historic and future outlook of this field was demonstrated.

2. Seminar Outcomes and Future Plan
   After his lecture, young researchers and students asked many questions and comments to Prof. Peng. For example, the details method to control the metal ion kinds and the number of difficulties in the synthetic procedure are essential for their experiments and studies. Furthermore, one researcher had interested in his compound for detailed magnetic investigations. This seminar was a good opportunity to start international collaboration.

Opening

Q&A

Prof. Shie-Ming Peng

Group Photo

3.Research achievements during his/her stay in Kumamoto University.

Prof. Peng demonstrated and taught the detailed experimental method and characterization process for making various coordination metal complexes possessing interesting metal-metal bonding. The Kumamoto univ students start the synthesis of related coordination metal complexes.

4. Prospect for further research collaboration.

His coordination metal complexes have the potential to exhibit quantum magnetism. Our group has one project to demonstrate such research, therefore we can do a collaboration with visiting professor.

IROAST Seminar & Research Activity Report by IROAST Visiting (Associate) Professor Invitation

No. 3-1-10 (Invitation Program) No. 4-2-8 (Seminar)	Name	Olivier BOUTIN	Title	Professor
	Affiliation	Aix-Marseille University, France		
Host Faculty	Name	Mitsuru SASAKI	Title	Associate Professor
	Affiliation	Institute of Industrial Nanomaterials（IINa）		
Seminar Title	92nd IROAST Seminar Subcritical water for waste treatment and biomass valorisation			
Style	Venue: International Seminar Room, 2F Kurokami South W4 (Faculty of Engineering Research Bldg. II)			
Time & Date	14:00-15:00, February 17, 2023			
Speaker's Name/ Title/Affiliation	Olivier Boutin, Professor, IROAST Visiting Professor Aix-Marseille University, France			
Number of Participants	Total: 9 (Int'l participants: 2) Invitees: 1 (Int'l participants: 1)			
Duration of Visit	From February 10, 2023-February 20, 2023			

1. Seminar Overview

The proposed seminar included 45 slides, for a presentation duration of 50 minutes.

The first part presents the University of Aix Marseille, the courses and the laboratory. M2P2 in which I work. This first part is also an opportunity to explain to the students present in the room the possibilities of exchange with the University of Aix Marseille, for semesters of courses or for periods of internship, in particular at the M2P2 laboratory.

In the second part, I wanted to address all the important elements for the understanding of the phenomena in subcritical and supercritical water, and the reasons why it is interesting and relevant to develop processes in these conditions.

The third and last part of this presentation first of all presents in a general way the different possibilities of implementing these processes for the treatment of organic matter, whether biomass or waste. The main difference lies in the presence or absence of an oxidant, and of course whether the fluid system is single-phase or two-phase. To illustrate these aspects, three examples from my latest research are proposed.

In conclusion, these different processes are highlighted in the context of the energy and ecological transition.

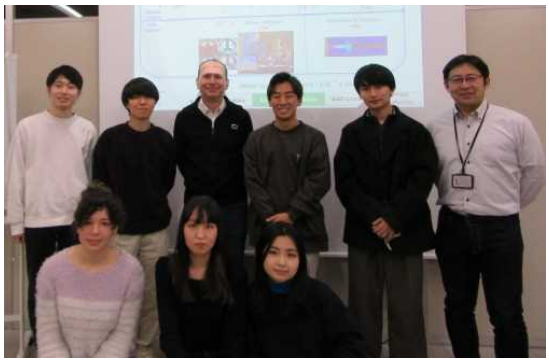
2. Seminar Outcomes and Future Plan (e.g. about contribution to the development of young researchers and the initiation of international collaborative research aiming for the publication of international collaborative papers, etc.)

As explained above, this seminar was an opportunity to show the possibilities of exchange with the University of Aix Marseille. Students are often reluctant to go abroad, in Europe, and I therefore emphasised the possibilities and the welcome provided by the University of Aix Marseille. On the other hand, on the research part, all the elements were provided, in particular on wet oxidation, allowing to put in perspective the research work which is currently carried out with Dr Sasaki.

Opening

Prof. Boutin

Q&A



Group Photo

3.Research achievements during his/her stay in Kumamoto University.

Despite the existence of wastewater treatment plants, many molecules can be released in trace amounts into the environment. Even at low or very low concentrations, some of these molecules still pose a risk to the environment in general and to humans in particular. Thus, traces of various pollutants such as industrial compounds, personal care products or endocrine disruptors are found in water at concentrations in the μg L^{-1} or ng L^{-1} range. Traces can also be found in drinking water, which has a direct impact on human beings. However, several studies indicate that the levels of endocrine disruptors in wastewater decrease after conventional biological treatment, mainly by simple adsorption onto activated sludge, which may then pose the problem of sludge management. Of all the compounds, this study focuses on the fate of bisphenol A. Bisphenol A (2,2-bis(4-hydroxyphenyl) propane; BPA) is used as a chemical intermediate in the manufacture of chemicals, such as polycarbonates, epoxy resins for can coating, powder coatings, adhesives, building materials and paper coatings. Bisphenol A is thus released into the environment through leaching from plastic waste and landfill leachate. It is acutely toxic at concentrations between 1 and 10 mg L^{-1} for marine species, as an endocrine disruptor causing various diseases, including cancer.

The objective of the work is to compare the treatment of BPA through wet air oxidation treatment and pulsed discharge treatment. Here are presented results on wet air oxidation.

Synthetic observation from bibliographical research

<u>Pub1</u> CWAO with materials based on activated carbon, CeO_2, TiO_2, MnO_2, ZrO_2, and their mixed oxides, which have been tested in the CWAO of phenol

100°C, air 20 bar, 10 mg/L

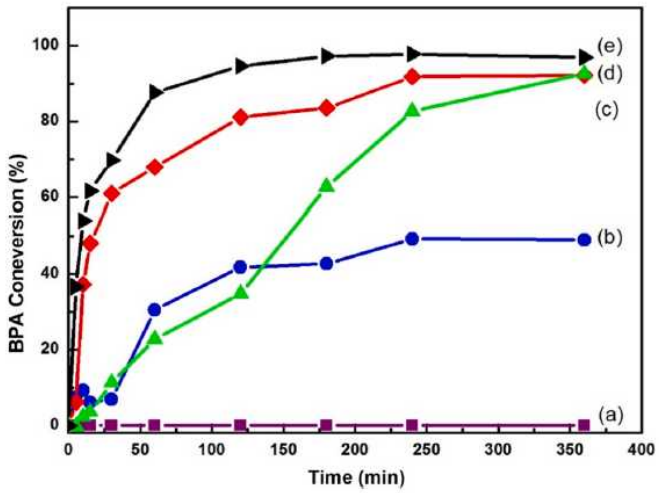


Fig. 8. BPA conversions as a function of time: (a) without catalyst,(b) $ZrO_{2\ C}$, (c)3%Pd/$ZrO_{2\ R}$, (d) 3%Pt/$ZrO_{2\ R}$ and (e) 3%Ru/$ZrO_{2\ R}$.

Table 2
Relevant parameters of oxidation kinetic of BPA.

Models	Catalyst	qe exp (mg/g)	qe cal (mg/g)	K_1 (L/min)	R^2	Chi-square
PFO	ZrO_2	6.76	5.98	0.012	0.919	0.598
	3%Ru/ZrO_{2R}	10.24	9.82	0.106	0.863	0.983
				K_2 (g/min. mg)		
PSO	ZrO_2	6.76	7.49	0.002	0.922	0.355
	3%Ru/ZrO_{2R}	10.24	10.36	0.016	0.932	0.341

<u>Pub2</u> Catalytic wet air oxidation of bisphenol A model solution in a trickle-bed reactor over titanate nanotube-based catalysts

Catalyse protonated titanate nanotubes

10 mg/L 10 bar 200°C

Residual BPA content :

HPLC apparatus (Spectra systemTM), isocratic analytical mode, 100 mm×4.6 mm BDS Hypersil C18 2.4 m column thermostated at 30 ◦C (UV detection at = 210 nm with a mobile phase of methanol (70%) and ultrapure water (30%) at a flow rate of 0.5 mL min^{-1}).

Perkin-Elmer (model Lambda 45) UV-Vis spectrophotometer for the residual concentrations of BPA in the aqueous-phase

Ion chromatography (IC) using DX-120 Dionex apparatus, in order to determine eventual CWAO intermediates.

TOC content measurements were carried out with an advanced TOC analyzer (Teledyne Tekmar, model Torch) equipped with a highpressure NDIR detector. A high-temperature catalytic oxidation (HTCO) method was applied (at 750◦C), which subtracted the measured inorganic carbon (IC) content from measured total carbon (TC) content.

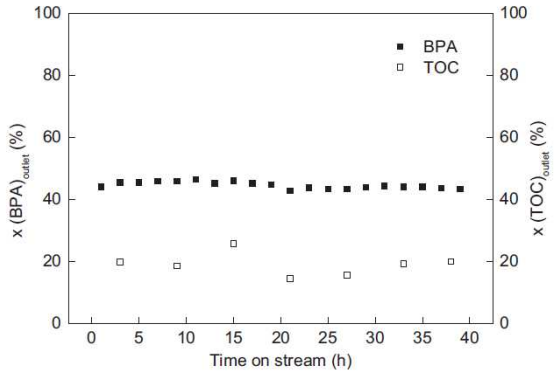


Fig. 7. BPA and TOC conversion as a function of time on stream obtained over SiC at 200 °C. Operating conditions: $p(O_2)$: 10.0 bar, $\Phi_{vol,L}$: 0.5 ml min^{-1}, $c(BPA)_{feed}$: 10.0 mg l^{-1}, T: 200 °C.

Results obtained with no catalysts

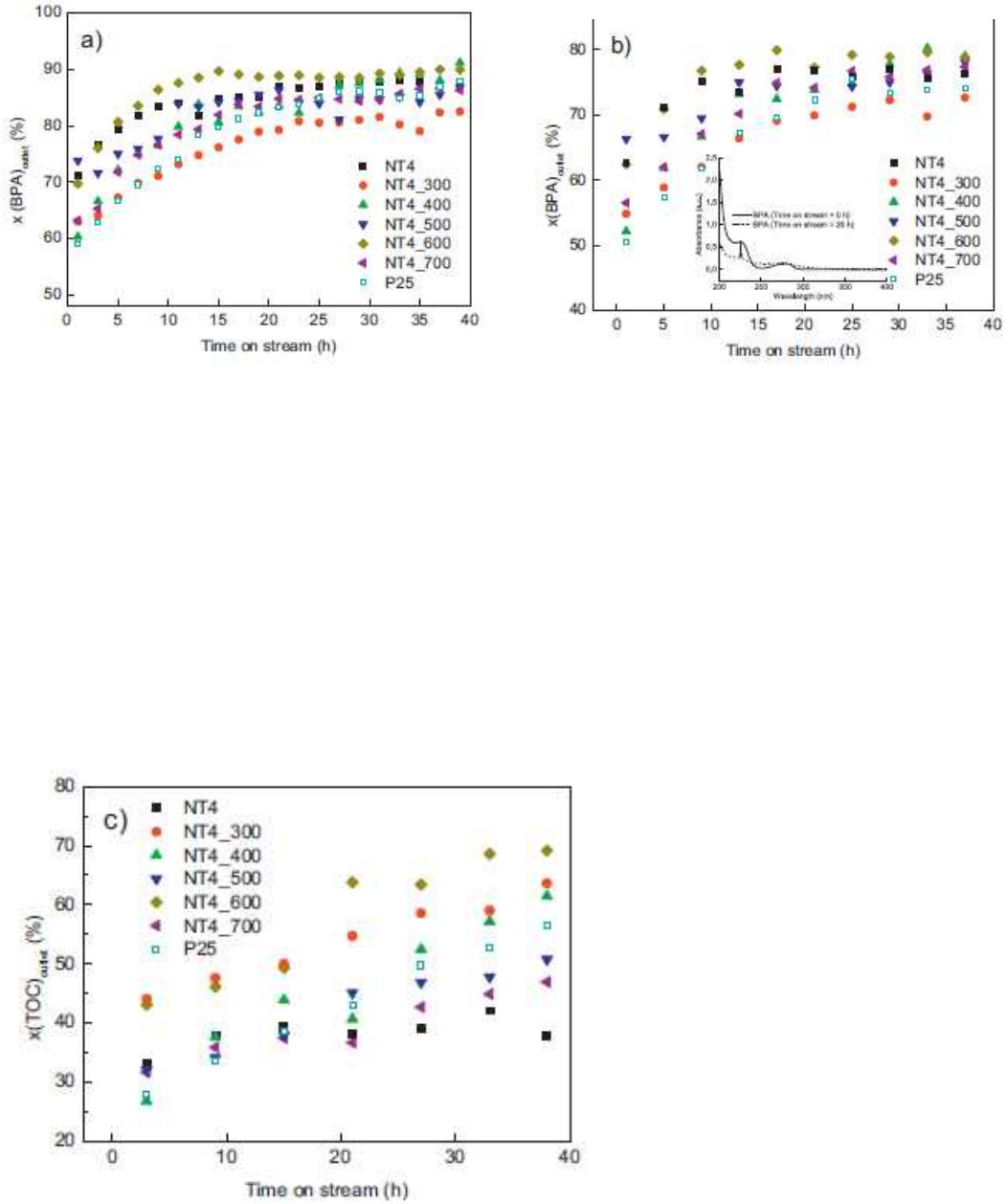


Fig. 8. BPA conversion as a function of time on stream over various titanate nanotube-based catalysts determined by means of (a) HPLC technique and (b) UV–vis spectroscopy, respectively. (c) TOC conversion as a function of time on stream over various titanate nanotube-based catalysts. Operating conditions: $p(O_2)$: 10.0 bar, $\Phi_{vol.}$: 0.5 ml min^{-1}, $c(BPA)_{feed}$: 10.0 mg l^{-1}, T: 200 °C.

Pub3 Magnetic titanium/carbon nanotube nanocomposite catalyst for oxidative degradation of Bisphenol A from high saline polycarbonate plant effluent using catalytic wet peroxide oxidation. Quantitative information's in this publication

Table 1

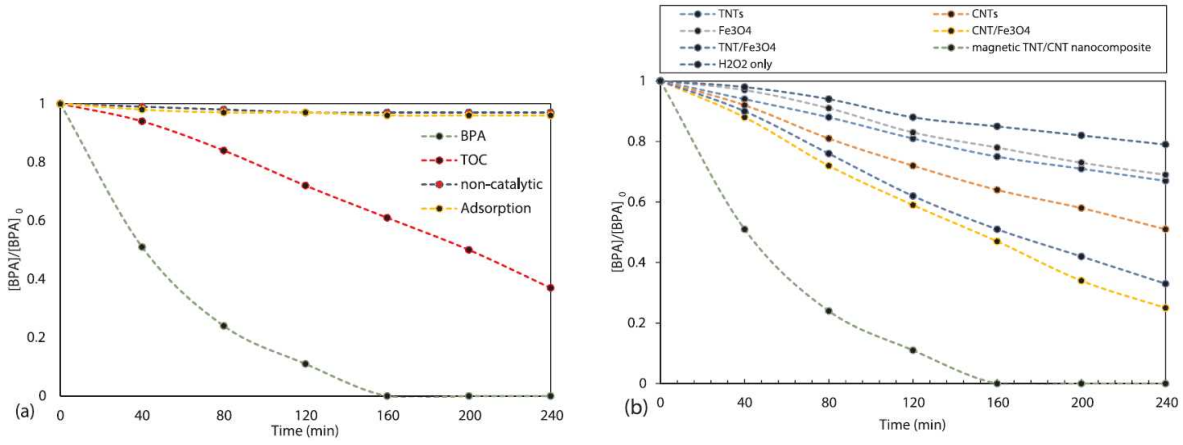
Characteristics of filtered raw high saline PCW, determined in triplicate measurements.

Parameter	Value	Unit
BPA (Bisphenol A)	50 ± 2	mgL^{-1}
COD (Chemical oxygen demand)	1650 ± 25	mgL^{-1}
BOD_5 (Biochemical oxygen demand)	255 ± 5	mgL^{-1}
BOD_5/COD	0.15 ± 0.02	–
Bicarbonate	10345 ± 155	mgL^{-1}
pH at 25 °C	8.6 ± 0.8	Sorensen scale
Conductivity	49510 ± 580	µS/cm
Chlorides	14395 ± 15	mgL^{-1}
TOC (Total organic carbon)	842 ± 110	mgL^{-1}
TSS (Total suspended solids)	63 ± 7	mgL^{-1}
TDS (Total dissolved solids)	25500 ± 14700	mgL^{-1}
Turbidity	24 ± 8	NTU
Appearance	Yellow	–

The concentration of BPA was analyzed by (HPLC, KNAUER, Germany), 2500 ultraviolet (UV) wavelength detector and a C18 (100–5) column (4.6mm×250 mm, with 5 µm particle size) as stationary phase, maintained at 35 °C in the oven. The UV detection wavelength for BPA was 214 nm. The mobile phase in an isocratic method was a mixture of Millipore water/acetonitrile with a 50:50 ratio at the flow rate of 1 mL min-1. 100 µL sample was filtered by Cellulose Acetate (CA) syringe filter (0.22 µm). retention time for BPA was 8.5 min. limit of detection was 0.01 mg L-1 and the limit of quantification was 0.1 mg L-1.

Agilent 7890 gas chromatograph with a 5975 single quadrupole mass spectrometer (Agilent,USA) (GC–MS analysis). HP-5MS capillary column (30m×0.25mm×0.25 µm, film thickness; Agilent, USA, 5% phenyl −95% Methyl Siloxane phase). splitting ratio of 10:1 in splitless mode at 280°C. carrier gas (Helium) constant flow rate of 1 mL/min. an initial temperature of 40°C (held for 1 min) was ramped at 5 °C/min to 300°C and held for 5 min. Post–run was3 min. Total GC–MS runtime was 56 min. The mass spectrometer was operated at EI mode at 70 eV. Selected compounds were identified by selected ion monitoring (SIM mode). Data was processed using MSD Chemstation-qualitative analysis software (Agilent Technologies).

Initial 600 mg L-1



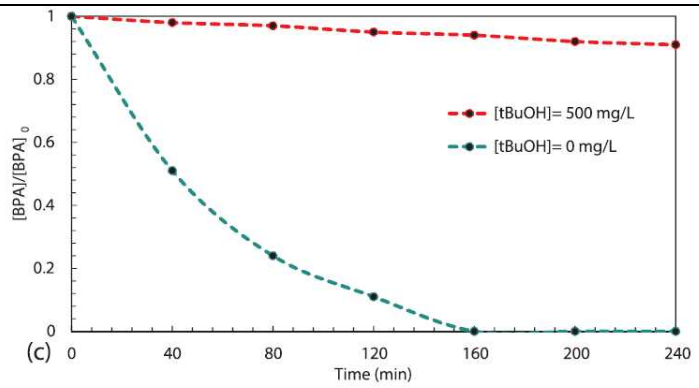


Fig. 5. CWPO of BPA using the magnetite TNT/CNT nanocomposite (a) BPA and TOC degradation (in aqueous solution) (b) comparison between catalytic performance of different catalysts in CWPO (c) effects of the presence of tBuOH in the BPA degradation. Experiments conducted under the conditions: $[BPA]_0 = 600$ mg/L, $[H_2O_2]_{stoichiometric} = 3.21$ g/L, pH = 3.5, T = 70 °C, catalyst loading = 50 mg/L.

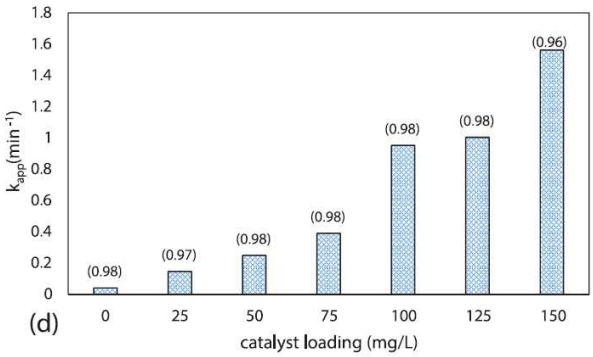
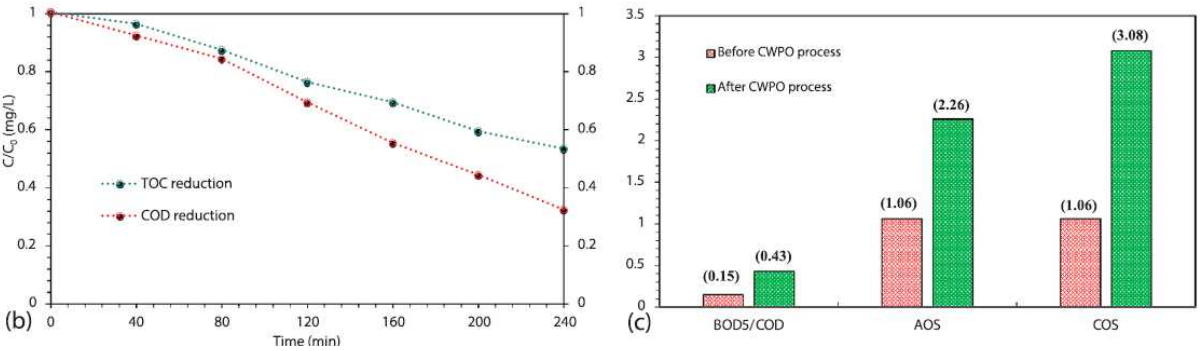


Fig. 8. Apparent first order reaction rate constants (k_{app}) obtained in CWPO experiments performed on the removal of BPA in the PCW under different (a) initial pH (b) H_2O_2 dosage (c) reaction temperature (d) catalyst loading. (The numbers in brackets represent the regression coefficients of the linear fitting (R^2)).

Table 2
The profile of the main organic compounds identified in the PCW effluent using qualitative GC/MS analysis.

Item code in GC/MS graph	Retention time (min)	Chemicals	Area (1 0 ^{4})		Removal Efficiency (%)
			Untreated	Treated	
1	14.73	2,4-Dichlorophenol	1.96	1.41	28.06
2	15.75	4,6-Dichlorophenol	3.31	2.35	29
3	17.69	Bisphenol, *tert*-butyldimethylsilyl ether	0.01	0.0	100
4	**18.31**	**Phenol, 4-(1,1-dimethylethyl)**	**0.15**	**0.17**	**–**
5	**18.75**	**2-Chloro-4-hydroxybenzonitrile 1,2,4-Trimethoxybenzene**	**0.16**	**0.44**	**–**
6	20.22	2,4,6-trichloro- phenol	58.04	45.60	21
7	22.14	2-Bromo-4,6-Dichlorophenol Thiophene	1.69	0.85	49
8	22.31	2-Bromo-4,6-Dichlorophenol Thiophene	1.56	0.97	37
9	**23.94**	**Phenol, 2,4-bis(1,1-dimethylethyl)**	**12.26**	**22.21**	**–**
10	24.13	2,6-Dichloro-4-(1,1-dimethylethyl) phenol	1.39	0.08	94
11	26.93	2H-2,4a-Methanonaphthalene, 1,3,4, 5,6,7-hexahydro-1,1,5,5-tetramethy l-	0.16	0.01	93
12	27.50	Silane, [[4-[1,2-bis[(trimethylsilyl)oxy]ethyl]-1,2-phenylene]bis(ox y)]bis [trimethyl-	0.62	0.16	74
13	29.57	3,5-di-*tert*-Butyl-4-hydroxybenzaldehyde	0.79	0.4	49
14	31.67	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	0.96	0.08	91
15	32.59	2,4,6-Trichlorophenol-Trimethyl-Silyl-Ether	1.16	0.1	91



On the contrary, if the BOD_5/COD ratio is below 0.4, it indicates the presence of toxic compounds in the effluent, which is considered to be not biodegradable or acclimated micro-organisms being required for its biological treatment [61]. The values of AOS and COS, as calculated based on Eqs. (21) and (22), are both ranging from −4 for methane as the most reduced state of carbon to +4 for carbon dioxide as the most oxidized state of carbon [1,13].

$$AOS = 4 - 1.5[COD/TOC] \quad (21)$$

$$COS = 4 - 1.5[COD/TOC_i] \quad (22)$$

<u>Pub4</u> Degradation of bisphenol A by electrocatalytic wet air oxidation process: Kinetic modeling, degradation pathway and performance assessment

HPLC, TOC, COD, BOD, GC-MS

The toxic effects of PPCPs and their degradation products evaluated by the inhibition growth of bacterium Escherichia coli in Luria-Bertani (LB) medium.

p-isopropenyl phenol and benzoquinone

Than propanedioic acid

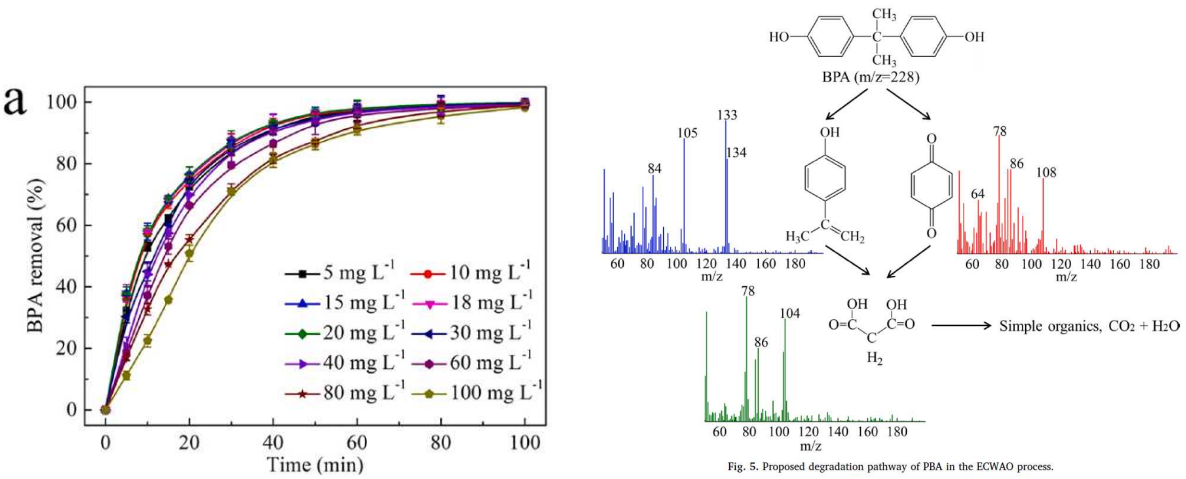


Fig. 5. Proposed degradation pathway of PBA in the ECWAO process.

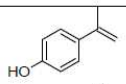
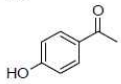
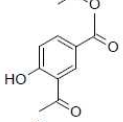
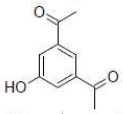
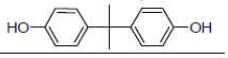
<u>Pub5</u> Catalytic wet air oxidation of bisphenol A aqueous solution in trickle-bed reactor over single TiO_2 polymorphs and their mixtures
Not interested

<u>Pub6</u> Efficient removal of bisphenol A from wastewaters: Catalytic wet air oxidation with Pt catalysts supported on Ce and Ce–Ti mixed oxides
HPLC, TOC, UPLC-MS (ultra performance liquide chromatography)
160°C, 2 MPa / dans ces conditions, pas de dégradation thermique après 3h

Table 7. BPA and TOC removal (±2.0%) after 3 h CWAO for C(100), CT(80) and CT(20) catalysts with and without Pt. Temperature 160 °C, air pressure 2.0 MPa, concentration of the catalyst 2 $g \cdot L^{-1}$.

Sample	BPA removal [%]	TOC removal [%]
C(100)	77	52
CT(80)	71	47
CT(20)	76	49
P/C(100)	97	59
P/CT(80)	95	60
P/CT(20)	90	58

Table 8. UPLC-MS data of the by-products detected in BPA solution treated by CWAO.

Compound	Molecular weight [$g \cdot mol^{-1}$]	Formula	Tentative structure
A	134	$C_9H_{10}O$	
B1	136	$C_8H_8O_2$	
B2	136	$C_8H_8O_2$	
C1	178	$C_{10}H_{10}O_3$	
C2	178	$C_{10}H_{10}O_3$	
BPA	227	$C_{15}H_{16}O_2$	

B et C are isomers molecules
A : 4-(prop-1-en-2-yl)phenol (same as previous publication)
B : p-hydroxyacetophenone
C1 : 1,1'-(4-hydroxy-1,3-phenylene)di(ethan-1-one)

<u>Pub7</u> Preparation of Granulated Biomass Carbon Catalysts—Structure Tailoring, Characterization, and Use in CatalyticWet Air Oxidation of Bisphenol A
HPLC with photo diode array detector

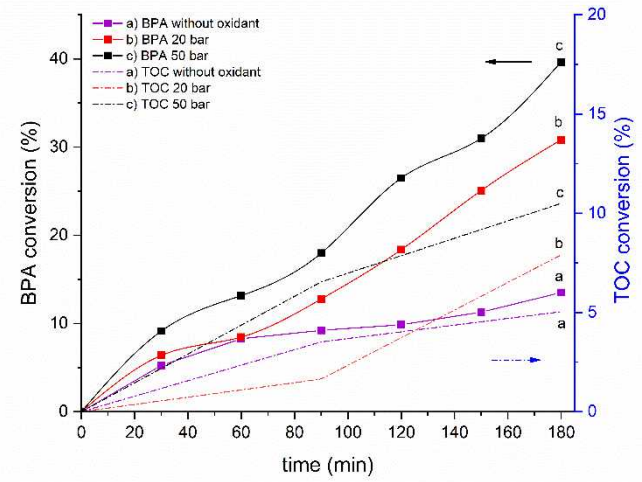


Figure 3. BPA and TOC conversion as a function of reaction time in non-catalytic experiments. Operating conditions: p (air): 20/50 bar, c (BPA): 60 mg/L, T: 160 °C, 800 rpm, pH initial 5–6. RSD ± 2%. Note the different scales on both y-axes.

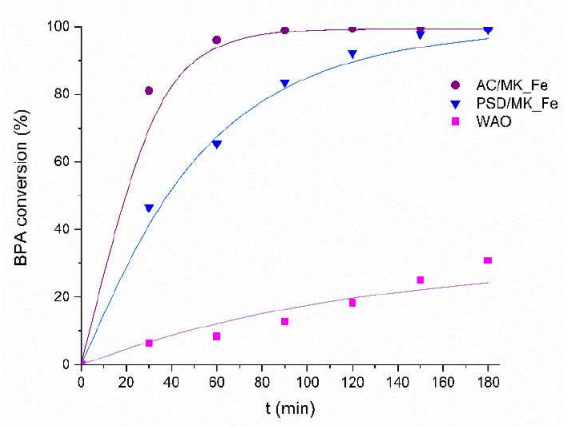


Figure 5. Bisphenol A conversion as a function of time for AC/MK_Fe and PSD/MK_Fe catalysts. Operating conditions: p (air): 20 bar, c (BPA): 60 mg/L, c (cat): 1 g/L, 800 rpm, T: 160 °C.

Pub8 Insights into the Kinetics Degradation of Bisphenol A byCatalyticWet Air Oxidation with Metals Supported onto Carbon Nanospheres

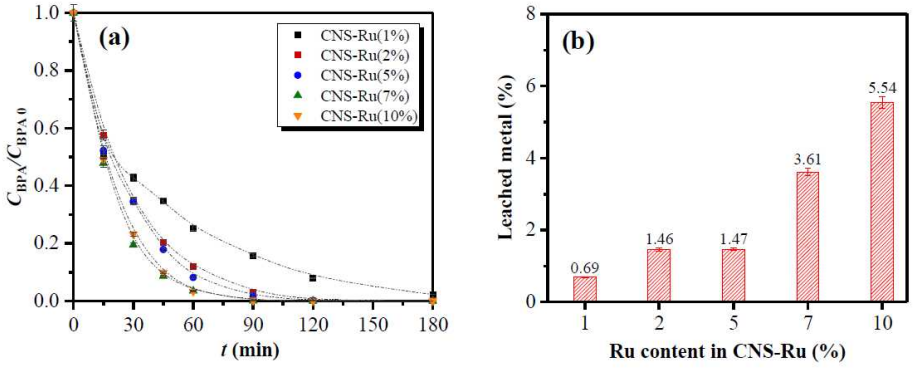


Figure 4. (**a**) Influence of the load of Ru in the BPA degradation (T = 130 °C, P = 20 bar, $[BPA]_0$ = 20 mg·L^{-1}, [CNS-Ru] = 2.0 g·L^{-1}, pH_0 = 7.0); (**b**) Percentage of leached ruthenium in the final reaction effluent measured at optimal conditions (T = 130 °C, P = 20 bar, $[BPA]_0$ = 20 mg·L^{-1}, [catalyst] = 2.0 g·L^{-1}, pH_0 = 7.0).

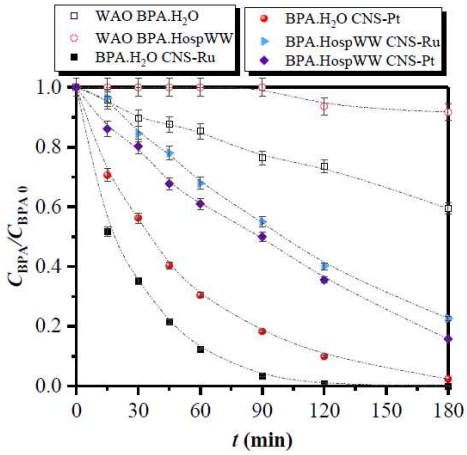


Figure 9. Degradation of BPA by WAO and CWAO solved in H_2O and HospWW at optimal conditions (130 °C, 20 bar, $[BPA]_0$ = 20 mg L^{-1} and 2.0 g·L^{-1} CNS-Ru).

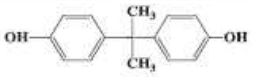
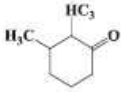
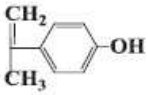
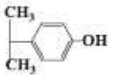
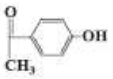
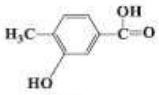
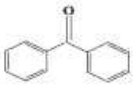
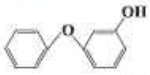
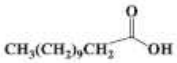
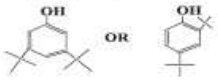
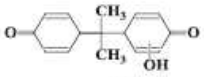
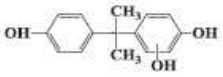
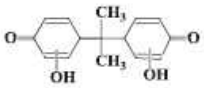
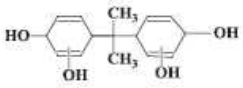
BPA oxidation mechanism

Oxidation2

Table 1
A brief overview of studies on the identification of by-products formed during the degradation of BPA.

Treatment method used	Operating conditions	Analysis method used	By products found	Remarks	Reference
Photo-catalysis	$C_0 = (170–175 \times 10^{-3}$ mM; TiO_2; 200-W Hg-Xe lamp (I_o = 10 mWcm^{-2})	LC/MS-MS; GC/MS	(m/z = 207; 133; 135; 145)	Four HPLC peaks appeared in Chromatograms monitored at 275 nm, all were disappeared after 20 h.	Ohko et al., 2001
Photo-Fenton oxidation	C_0 = 0.04 mM; $[Fe(II)]_0 = 4 \times 10^{-5}$ mol/l; $[H_2O_2]_0 = 4 \times 10^{-4}$ mol/l; pH 4.0	GC-MS; LC-MS	(m/z = 108; 94; 134; 110; 136)	The intermediates were formed by the photo cleavage of phenyl groups in BPA by attack of HO˙ radicals.	Katsumata et al., 2004
Ferrate oxidation	C_0 = 0.1 mM; $[Fe(VI)]_0$ = 0.05–0.5 mM)	LC/MS-MS; GC/MS-MS	(m/z = 134; 136; 152; 104; 208)	The oxidation of BPA initially starts at phenyl groups due to high electron density.	Li et al., 2008
Ozonation	$C_0 = 100 \times 10^{-3}$ mM; $[Ozone]_0$ = 15 −400 μM, pH = 6.5; Temp. = 20 °C	LC-UV; LC-MS; MS/MS	(m/z = 275; 151; 241; 243; 325; 459)	Ozone reaction by electrophilic substitution or 1, 3-dipolar cyclo addition.	Deborde et al., 2008
Sub-stoichiometric Fenton oxidation	$C_0 = 44 \times 10^{-3}$ mM; $[Fe^{2+}]_0/[BPA]_0$ molar ratio = 0.23 and 0.45, $[H_2O_2]_0/[Fe^{2+}]_0$ = 10; pH = 3	GC/MS	(m/z = 90; 94; 108; 110; 136; 164; 242; 244; 270; 276; 258; 302) Coupling products (m/z = 336; 320; 362; 350; 454; 470)	The HCHD radical played central role. Larger molecular weight compounds were formed due to: • oxidative coupling reactions of stabilized free radicals • addition of organo-radicals to BPA molecules or benzene-diols.	Poerschmann et al., 2010
ϒ-radiation induced oxidation	C_0 = 0.08 mM; Radiation source: ^{60}Co, @7.4 × 10^{14} Bq.	GC-MS	m/z values were not reported	o-MHBPA; m-MHBPA; HO˙ radical attack was responsible for oxidation	Guo et al., 2012
HO˙, $SO_4^{-\cdot}$ and $CO_3^{-\cdot}$/HCO_3^{-} radicals	C_0 = 0.04 mM; MPUV P = 700 W, ($I_o = 5.74 \times 10^{-5}$ E s^{-1}) $[H_2O_2]_0 = [K_2S_2O_8]_0 = [Na_2CO_3]_0$ = 500 μM, Temp. = 25 °C	UPLC-MS	m/z values were not reported	Using UV/H_2O_2 and UV/Na_2CO_3 = MHBPA, Q-MHBPA. Using UV/$K_2S_2O_8$ = 4-isopropenylphenol, mono-hydroxylated 4-iso-propenylphenol; $SO_4^{-\cdot}$ attacks BPA through the dimethylated carbon atom and leads to fragmentation	Sanchez-Polo et al., 2013
Photocatalysis	C_0 = 0.02 mM; $H_3PW_{12}O_{40}/TiO_2$ catalyst; $H_3PW_{12}O_{40}$ loading 6.3%	HPLC-MS	(m/z = 151, 121, 109, 137, 93)	HO˙ attacks the electron rich C_2 of BPA followed by cleavage of two phenyl groups	Lu et al., 2013
Thermally activated persulfate	C_0 = 0.08 mM; Temp. = 40,50,60,70 °C; $[K_2S_2O_8]_0$ = (0–20 mM); pH = 6.5	GC-MS	(m/z = 90; 106; 118; 134; 150; 152; 281; 355; 362; 415; 429; 502)	Hydroxylation and coupling reactions said to be responsible for degradation	Olmez-Hanci et al., 2013
Photo-fenton like oxidation	C_0 = 0.22 mM; Fe^{3+} = 0.20 mM; H_2O_2 = 4.0 mM	GC-MS	(m/z = 110; 128; 140; 162; 134; 136; 202; 150; 214; 277; 218)	Reaction pathway based on hydroxylation, dimerization and ring opening steps	Molkenthin et al., 2013
Ferrous ion activated persulfate	$C_0 = 80 \times 10^{-3}$ mM; $(S_2O_8^{2-})$ = 2 mM (Fe^{2+}) = 1.6 mM	LC/MS	(m/z = 136; 242)	Electrophillic attack of sulfate radicals was responsible for degradation.	Jiang et al., 2013
Chemical oxidation	$C_0 = 25 \times 10^{-3}$ mM; permanganate $[Mn(VII)]_0$ = 250 μM. Temp. = 20 C; pH = 7	LC-MS/MS	(m/z = 244; 242; 276; 136; 152).	Permanganate oxidized phenolic compounds via [3 + 2] addition, followed by a hydride abstraction from the substrate to permanganate oxo group	Zhang et al., 2013
Fenton-like oxidation: H_2O_2 activated by $CuFeO_2$	C_0 = 0.1 mM; $[H_2O_2]_0$ = 20 mM, $[CuFeO_2]_0$ = 1.0 g/l, pH = 5.0	GC-MS	(m/z = 94; 134; 110; 136; 244)	$CuFeO_2$ is more effective than Cu_2O and Fe_3O_4 in H_2O_2 activation; HO˙ attack on the middle carbon atom introduces cleavage between benzene rings and the isopropyl group	Zhang et al., 2014
Photo-chemical oxidation using PMS	C_0 = 0.22 mM $[PMS]_0$ = 0.66 mM; pH = 5.15	HPLC, GC-MS, FTIR	(m/z = 116,168, 186, 242, 244, 206, 257, 270)	The degradation products formed reveals the electron (e^-) transfer mechanism as $SO_4^{-\cdot}$ radicals attack was predominant	Sharma et al., 2015b
Photo-chemical oxidation using H_2O_2, $Na_2S_2O_8$	C_0 = 0.22 mM; $[H_2O_2]_0$ = 11.76 mM, $[Na_2S_2O_8]_0$ = 1.26 mM, pH = 5.0	HPLC, GC-MS, FTIR	(m/z=257,242,206, 186,152,136,134,320) $SO_4^{-\cdot}$ (m/z = 262, 244, 206, 182, 286) HO˙	The addition mechanism in HO˙ radicals attack and e-transfer mechanism in $SO_4^{-\cdot}$ radicals attacks found to be responsible for the formation of hydroxylated products of BPA and quinone of BPA.	Present study

Table 3
The intermediates identified during BPA treatment using UV-C/H_2O_2 and UV-C/SPS system.

Compound	Structure	MW	Oxidation process	
			UV-C/SPS	UV-C/H_2O_2
Bisphenol-A		228		
Dimethylcyclohexane		126		√
p-isopropenylphenol		134	√	
p-isopropylphenol		136	√	
p-hydroxyacetophenone		136	√	
3-hydroxy-4-methyl benzoic acid		152	√	
Benzophenone		182		√
Pentadecanoic acid pentyl ester	$C_{10}H_{18}O_3$	186		√
Hydroxy diphenyl ether		186	√	
Dodecanoic acid		200		√
Phenol, bis(dimethyl ethyl) isomers		206	√	√
Q-MHBPA		242	√	
MHBPA		244		√
Q-DHBPA		257	√	
DHBPA		262		√

MHBPA = monohydroxylated BPA, Q-MHBPA = quinone of monohydroxylated BPA, DHBPA = dihydroxylated BPA, Q-DHBPA = quinone of dihydroxylated BPA.

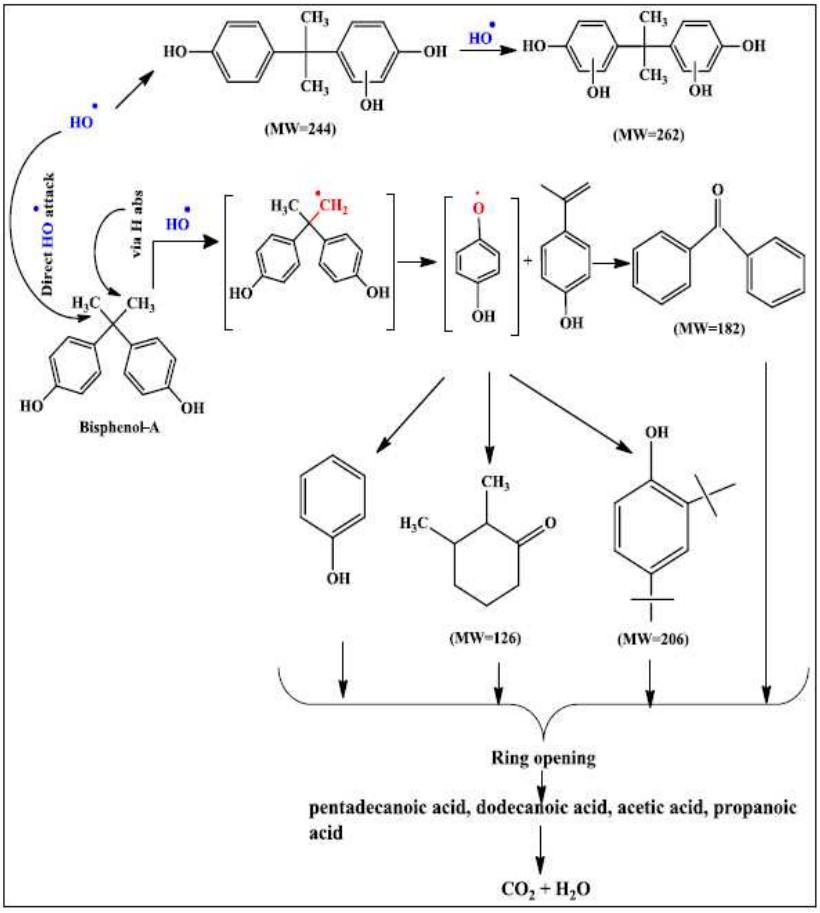


Fig. 6. Proposed degradation mechanism of BPA under HO˙ radical attack.

Oxidation3

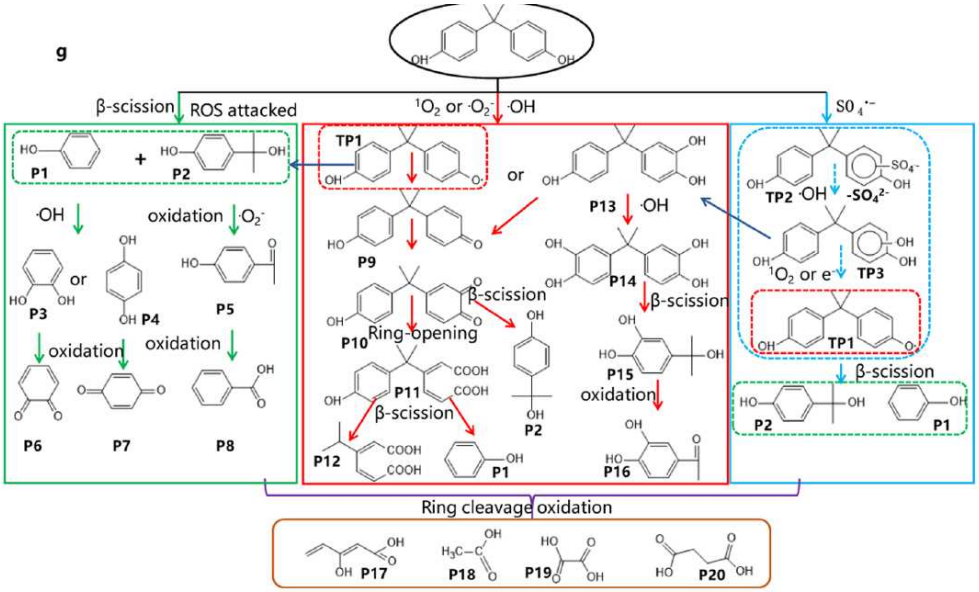
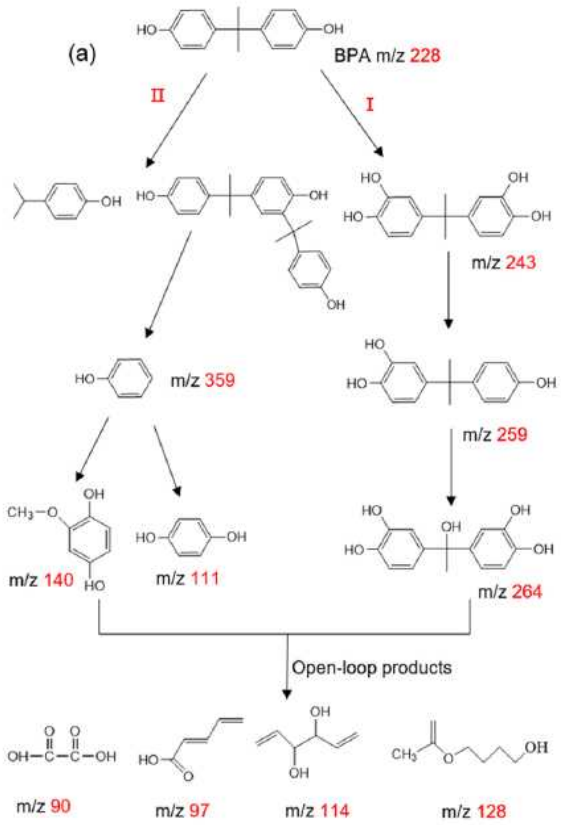


Fig. 8. (a) Optimized structure and numbering system for the BPA, (b) electrostatic potential (ESP) surfaces of BPA, (c) HOMO and (d) LUMO distributions of BPA, (e) the Fukui index (f^-) representing the nucleophilic sites of BPA, (f) isopleth image of the Fukui function (Δf) for BPA (green and blue isosurfaces represent positive and negative parts, respectively), and (g) possible degradation pathways for BPA in the FeBCG/PS system.

Oxidation5

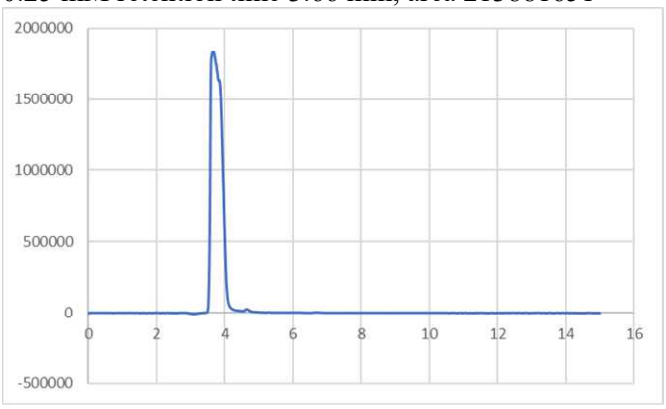


Experiments through WAO made at Aix Marseille University
Prepare a 1L solution at 100 mg per litre. Wear a protective mask.
Make a TOC measurement on this initial solution.
For all tests, note the times (rise, fall, etc.), temperatures and pressures. Stir at 700 rpm for all tests.
Each test starts with 100 mL of solution, atmospheric pressure, inerted with nitrogen. After each test, make a TOC measurement and store the rest in the refrigerator.
Test 1: heat to 300°C, then cool (no oxidation).
For the following tests, with oxidation, increase the temperature, note the pressure, and complete with air to reach 150 bar. Leave for the duration of the stage and then cool down.
Test 2: 200°C, 30 min
Test 3: 250°C, 30 min
Test 4: 300°C, 30 min
Test 5: 300°C, 60 min
Test 6: 300°C, 30 min, with an initial sample diluted 1 time (50mL solution°50mL water)

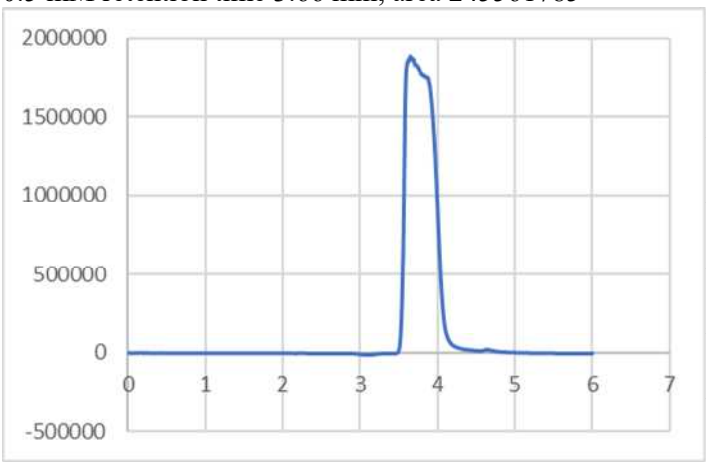
Results obtained through HPLC measurements made at Kumamoto University
Analyses HPLC InertSustain C18
35°C
Detector Jasco MD-4017 Photo Diode Array Detector (200-400 nm)
1 mL/min
Acetone/distilled water 1 :1
20 □L
200 nm
For hydroquinone, benzoquinone …

Results on pure hydroquinone

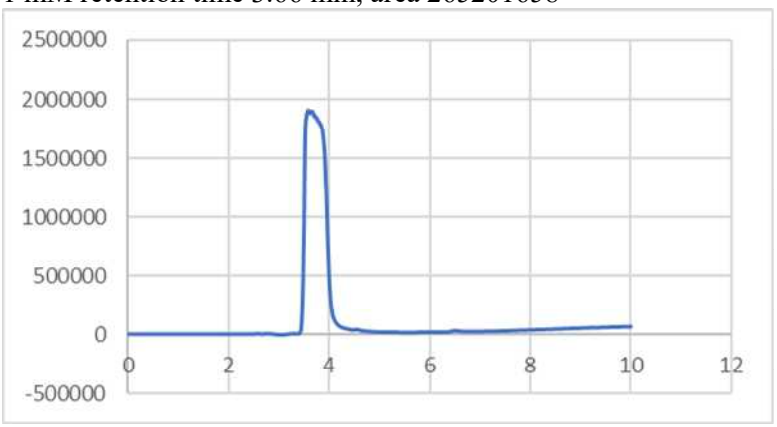
0.25 mM retention time 3.66 min, area 213881651



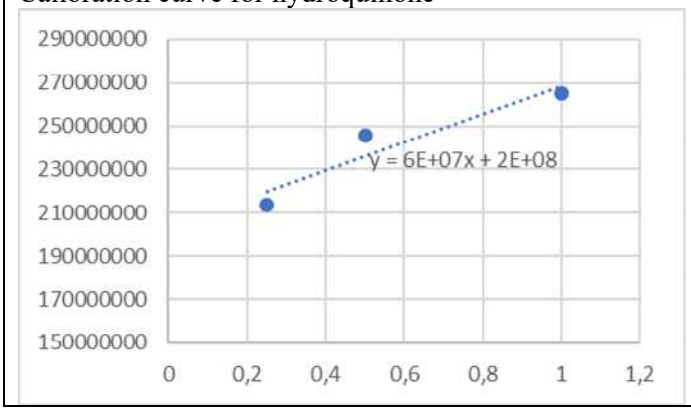
0.5 mM retention time 3.66 min, area 245561785



1 mM retention time 3.66 min, area 265201658

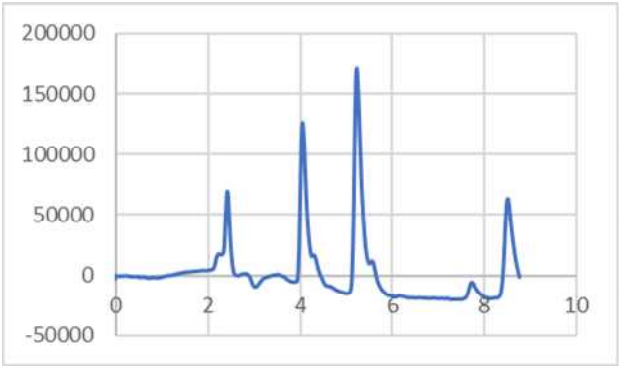


Calibration curve for hydroquinone

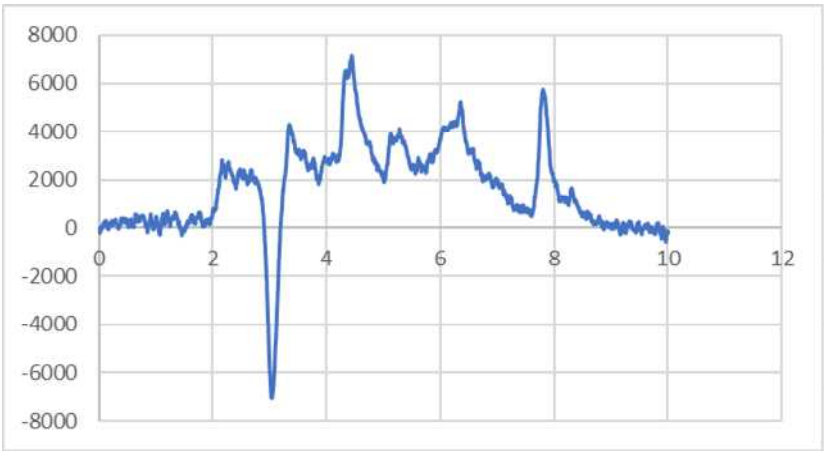


HPLC results for WAO experiments

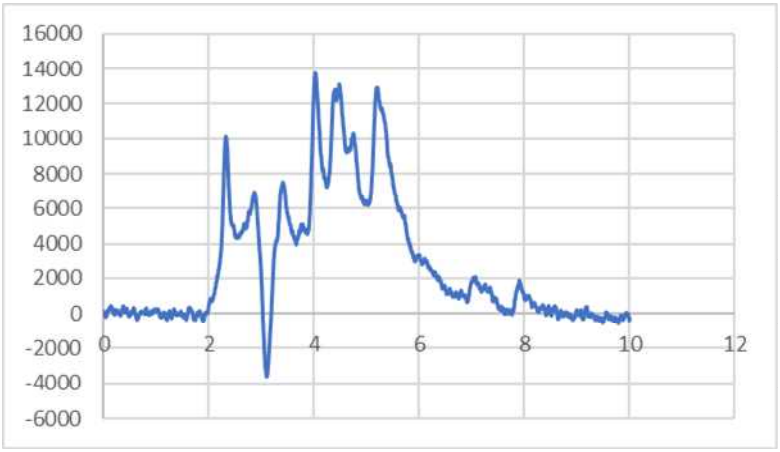
Test 1



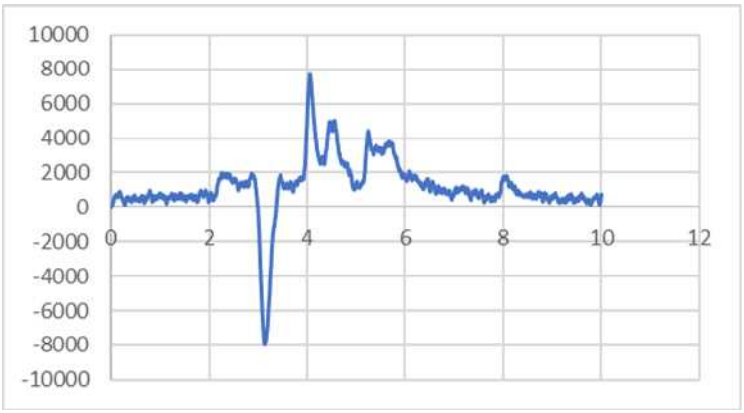
Test2



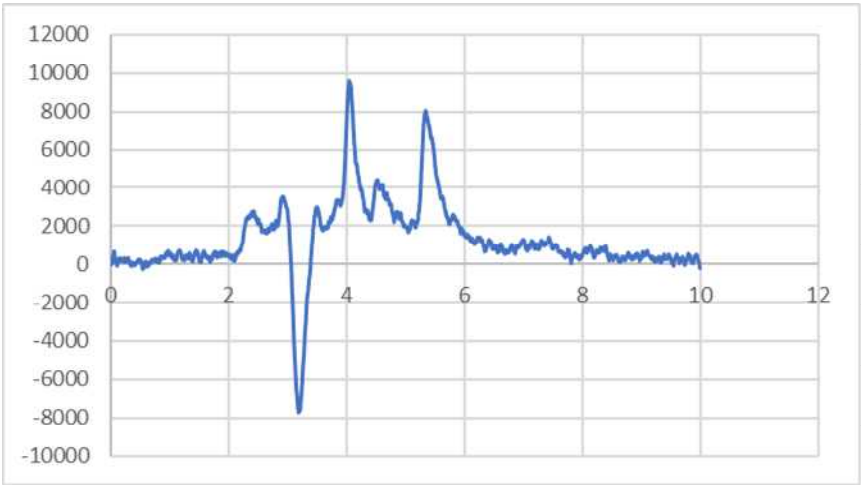
Test3



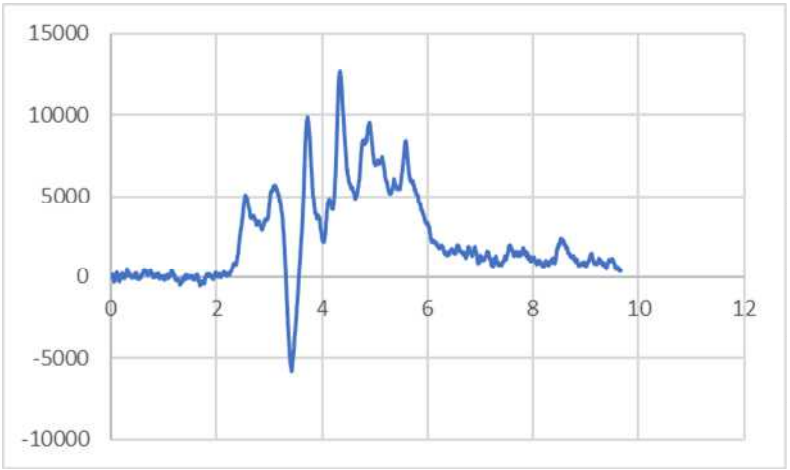
Test4



Test5



Test 6



4. Prospect for further research collaboration.

For further work, we need to calibrate and evaluate the different analysis through LC-MS proposed by Dr Sasaki.

I will have the final results from COT measurements.

After that, we need the results from pulsed discharge experiments to start the comparison between both processes.

IROAST Seminar & Research Activity Report by IROAST Visiting (Associate) Professor Invitation

No.3-1-11 (Invitation Program) No.4-2-9 (Seminar)	Name	Dario ZAPPA	Title	Associate Professor
	Affiliation	The University of Brescia, Italy		
Host Faculty	Name	Tetsuya KIDA	Title	Professor
	Affiliation	Faculty of Advanced Scient and Technology (FAST)		
Seminar Title	93rd IROAST Seminar Metal oxide nanostructures as building blocks for energy and environmental application			
Venue	Kurokami South W4 (Faculty of Engineering Research Bldg. II) 2F Conference Room			
Time & Date	16:00-17:00, March 1, 2023			
Speaker's Name/ Title/Affiliation	Dario Zappa, Associate Professor, The University of Brescia, Italy			
Number of Participants	Total: 31 (Int'l participants: 16) Invitees: 1 (Int'l participants: 1)			
Duration of Visit	From February 28, 2023- March 6, 2023			

1. Seminar Overview

In the seminar, Prof. Dario Zappa talked about the synthesis of one-dimensional nanomaterials and their applications in the energy and environmental fields. He gave examples of metal oxide nanostructures (nanowires, nanotubes, surface-functionalized nanowires, and heterostructures) and explored their potential use as chemical sensors and for the production of solid oxide fuel cells. Various growth and characterization techniques have proven effective in tailoring the properties of materials to specific applications. In addition, several strategies for improving the sensitivity and selectivity of metal oxide chemosensors were discussed. The formation of p-n junctions between nanostructures significantly improved device performance.

2. Seminar Outcomes and Future Plan

The seminar broadened the perspectives of the participating researchers and students on the science and technology of fuel cells and gas sensors using metal oxide nanowires. Before and after the seminar, the possibility of future collaborative research and international joint publications were discussed. Plans for student exchange programs were also agreed upon. The host professor plans to send two graduate students to Brescia to conduct joint research.

Dr. Dario Zappa

Group Photo


93rd IROAST Seminar
Wed,March 1, 2023 16:00-17:00
@ Kurokami South W4
(Faculty of Engineering Research Bldg. II)
2F Conference Room
Metal oxide nanostructures as building blocks for energy and environmental applications
Dr. Dario Zappa
Assoc. Prof.,The University of Brescia, Italy
Organizer: Prof. Tetsuya Kida, FAST
Contact: IROAST Phone: 096-342-3362 E-mail: szk-kiko@jimu.kumamoto-u.ac.jp
Web: http://iroast.kumamoto-u.ac.jp/