2019 Joint Workshop on Environmental Science

March 18-21, 2019
Hong Kong Baptist University
Hong Kong SAR, China

Presented by

HKBU-RCEES Joint Institute of Environmental Sciences

環境與生物分析國家重點實驗室
State Key Laboratory of
Environmental and Biological Analysis

环境化学与生态毒理学
国家重点实验室
State Key Laboratory of Environmental
Chemistry and Ecotoxicology

Program of Scientific Presentations

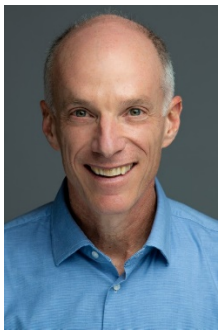
Date: March 19, 2019 (Tuesday)

Venue: RRS905, Sir Run Run Shaw Bldg, Hong Kong Baptist University

Time	**Topic**	**Speaker**	**Chair Person**
9：00 - 9：05	Welcome Speech	Guibin Jiang	Zongwei Cai
9：05 - 9：35	Formation and Fate of Aldehydes and Dicarbonyl Compounds During Oxidative Water Treatment	David Sedlak	Guibin Jiang
9：35 - 10：05	Toxicology and Health Risks of PM2.5	Guibin Jiang	Xiangdong Li
10：05 - 10：25	Microfluidic Analytical System for Rapid Survey of Antimicrobial Resistance in Environmental Microorganisms	Kangning Ren	
10：25 - 10：40	Stem Cell Toxicology: A Powerful Tool For Comprehensive Developmental Toxicity Evaluations	Nuoya Yin	
10：40 - 11：00	Group Photo & Tea Break		
11：00 - 11：20	Mechanism for Preventing and Treating Oral Leukoplakia Carcinogenesis by Ruthenium Complex	Benzhan Zhu	Minghui Zheng
11：20 - 11：40	DTT Activity And ROS Generation Ability Of Water-Soluble PM2.5 In Hong Kong: Characterization And Source Apportionment	Di Hu	
11：40 - 12：00	Arsenic Adsorptive Removal Using TiO_2	Chuanyong Jing	
12：00 - 12：20	Exposure to BDE-47 Promotes Obesity and Aggravates Liver Dysfunction in Diet-Induced Obesity Mice	Chi Kong Chung	
12：20 - 12：40	Profiling of DNA Modifications for Epigenetics	Hailin Wang	
12：40 - 14：20	Lunch（Refrew Restaurant）		
14：20 - 14：40	Separation and Determination of Trace Nanoparticles in Complex Matrices	Jingfu Liu	
14：40 - 15：00	Effects of PFOS on the Gut Microbiome and Metabolic Profiles in Mice	Yanjun Hong	

15：00 - 15：20	PFASs Exposure Relates to Oxidative Stress, Fatty Acid β-Oxidation Disorder, and Potential Kidney Injury in Occupational Workers in a Manufactory in China	Yawei Wang	Benzhan Zhu
15：20- 15：40	Porphyrin-Implanted Carbon Nanodots for Photoacoustic Imaging and cancer therapy	Xunjin Zhu	
15：40 - 16：00	Seasonal Variation and Human Exposure Assessment of Legacy and Novel Brominated Flame Retardants in $PM_{2.5}$ in Different Microenvironments in Beijing, China	Qinghua Zhang	
16：00 - 16：10	Tea Break		
16：10 - 16：30	Silver Nanoparticles Impair Generation of Amputated Zebrafish Fins	Maoyong Song	Di Hu
16：30 - 16：50	3D Printing of Devices for Chemical Analysis	Ligang Hu	
16：50 - 17：05	Airborne Fine Particulate Matter Induces Cognitive and Emotional Disorders in Offspring Mice Exposed During Pregnancy	Chao Zhao	
17：05 - 17：20	Integration of Metabolomics and Lipidomics Reveals Metabolic Mechanisms of Triclosan-Induced Toxicity in Human Hepatocytes	Hongna Zhang	
17：20 - 17：35	Toxicity of Black Phosphorus Nanosheet	Guangbo Qu	
17：35 - 17：50	The Health Risk of Environmental Pollutants Exposure and Metabolomics Study on Pregnant Disease	Hongzhi Zhao	
17：50 - 18：05	Chemodiversity and Interfacial Behavior of Dissolved Organic Matter	Jitao Lv	
18：05 - 18：20	Molecular Characterization of Natural Organic Matter by ESI-Fourier Transform Ion Cyclotron Resonance Mass Spectrometry	Dong Cao	
18：20 - 18：40	Non-Targeted Screening of Organic Pollutants in $PM_{2.5}$ by Comprehensive Two-Dimensional Gas Chromatography Coupled with High Resolution Time-of-Flight Mass Spectrometry	Minghui Zheng	
19：00 - 20：30	Dinner (Sai Kung Hung Kee Seafood Restaurant)		

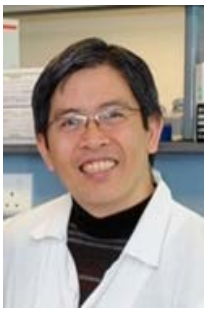
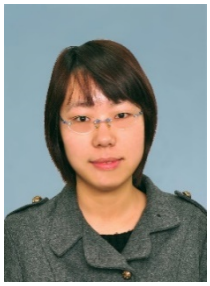
Biography

	**David Sedlak** Professor David Sedlak is the Plato Malozemoff Professor in the Department of Civil & Environmental Engineering at UC Berkeley. He is a member of the US National Academy of Engineering and Editor-in-Chief of *Environmental Science & Technology*. His research interests include oxidative water treatment technology, potable water reuse and natural water treatment systems. He is currently a visiting professor at The Hong Kong Polytechnic University.
	**Guibin Jiang** Professor Guibin Jiang, member of Chinese Academy of Sciences and a fellow of the Third World Academy of Sciences. His research is mainly focused on Environmental Chemistry and Toxicology. He has published 700 articles in leading scientific journals. He is also the author of 14 scientific books. As an invited plenary or keynote speaker, he has presented in more than 590 times at international meetings, institutes and universities. He is the recipient, in three times, of the prize of National Natural Science Award.
	**Minghui Zheng** Professor Minghui Zheng, deputy director of State Key Laboratory of Environmental Chemistry and Ecotoxicology. He is a leading expert on POPs monitoring in China. He also contributes to international POPs monitoring activities for the the effectiveness evaluation under the Stockholm Convention. He is a Coordinator of Asia-Pacific Regional Organization Group for POPs monitoring (2007-). He has published more than 200 scientific papers in peer reviewed journals.
	**Benzhan Zhu** Prof. Benzhan Zhu, co-director of Joint Institute of Environmental Science between RCEES and HKBU. He is the winner of the NSFC “Distinguished Young Scholars”. His major researches are a novel mechanism for the production of hydroxyl and alkoxyl radicals by the carcinogenic halogenated quinones (XQs) and hydroperoxides, which is different from the classic Fenton reaction.

	**Chuanyong Jing** Prof. Chuanyong Jing, deputy director of State Key Laboratory of Environmental Chemistry and Ecotoxicology. He is the winner of the NSFC “Distinguished Young Scholars”. His research primarily focuses on the areas of environmental molecular and interface science. Key areas of his investigation include biogeochemical cycles of environmentally significant trace elements including arsenic and antimony, and environmental remediation using nanotechnology.
	**Hailin Wang** Prof. Hailin Wang, the winner of the NSFC “Distinguished Young Scholars”. He has his expertise in epigenetics, in particular, DNA methylation and demethylation. He is a pioneer for the discovery of DNA N6-methyladenine in high eukaryotes.
	**Jingfu Liu** Prof. Jingfu Liu, the winner of the NSFC “Distinguished Young Scholars”. His major research interests involve the environmental analysis, processes and effects of persistent toxic substances and nanoparticles. He has published over 230 peer-reviewed papers in leading journals. He received twice Second Prizes of the National Natural Science Award (2018, 2011).
	**Yawei Wang** Prof. Yawei Wang, deputy director of State key Laboratory of Environmental Chemistry and Ecotoxicology. He is the winner of the NSFC “Distinguished Young Scholars”. His research interests are analytical methodology, environmental behavior and transformation of new persistent organic pollutants.
	**Qinghua Zhang** Prof. Qinghua Zhang, director of instrumental analysis laboratory of RCEES. His research focuses on developing sampling and analytical methods for persistent organic pollutants (POPs) and investigating sources, process and impact of POPs in China and polar regions.

	**Maoyong Song** Professor Maoyong Song, deputy director of Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences. He is the winner of the NSFC “Outstanding Yong Scientist”. In the recent few years, Prof. Song has mostly investigated the toxicological mechanisms of nanoparticles and emerging chemicals in cell and animal models. He has published more than 50 papers in peer-reviewed leading journals.
	**Ligang Hu** Prof. Ligang Hu, the winner of “The Thousand Talents Plan for Young Professionals”. His current research interests involve metallomics, environmental health (with focus of heavy metals) and biogeochemical cycling of metals.
	**Guangbo Qu** Prof. Guangbo Qu, the winner of the NSFC “Outstanding Yong Scientist”. His Current research directions include (1) developing high throughput multiple target assay for the screening of environmental contaminants; (2) identification of main toxic pollutant in environmental compartments using effect-directed analysis; (3) elucidating the mechanism underlying the biological effect of nanomaterials.
	**Nuoya Yin** Dr. Nuoya Yin, associate professor at the Stem Cell Toxicology Group, SKLECE. In the past few years, she was mainly focused on the neurotoxicological evaluation of several environmental pollutants, such as bisphenols, perfluorinated compounds and nanoparticles. Recently, she has set up a global differentiation model based on human embryonic stem cells and employed it for the assessment of pollutants' developmental toxicity and their link to diseases.
	**Jitao Lv** Dr. Jitao Lv, an associate professor at State Key Laboratory of Environmental Chemistry and Ecotoxicology. His research interests focus on the environmental geochemical behaviors of natural organic matters, nanominerals and persistent toxic substances.

	**Dong Cao** Dr. Dong Cao, a senior engineer at the State Key Laboratory of Environmental Chemistry and Ecotoxicology. His research mainly focuses on analysis of unknown compounds in environmental complex mixture by FTICR-MS methods.
	**Kangning Ren** Dr. Kangning Ren obtained both his Bachelor's and Doctor's degree from Tsinghua University, with a major in Chemistry. In June 2008, he came to Hong Kong and worked as a postdoc for three years in Department of Chemistry. From July 2011 to August 2014, he conducted research at Stanford University. In September 2014, he joined HKBU as assistant professor in the department of Chemistry. In 2016, he joined the State Key Laboratory of Biology and Environmental Analysis as an academic member. His current research interests center on functional materials and advanced analytical chemistry technologies, with particular emphasis on materials engineering and analytical technologies based on microfluidics.
	**Di Hu** Dr. Di Hu is an assistant professor in the Department of Chemistry, Hong Kong Baptist University. She is also an academic member in the SKLBEA. Dr. Hu obtained her B.Sc. degree from Peking University and Ph.D. degree from the University of North Carolina at Chapel Hill, USA. Her current research interests are: 1) characterization and source apportionment of organic aerosols and PM-associated toxicity; 2) formation mechanisms of secondary organic aerosol.
	**Xunjin Zhu** Dr. Xunjin Zhu obtained his PhD in 2006 from Hong Kong Baptist University and is currently an Assistant Professor of the Department of Chemistry at Hong Kong Baptist University. His current research interests focus on some interdisciplinary research topics, including the design and synthesis of new porphyrin-based small molecules for solar-to-electricity conversion in photovoltaics, solar-to-chemical conversion in photocatalytic water-splitting, CO2 reduction and photoredox catalysis; new porphyrin (phthalocyanine) implanted nanodots for photoacoustic imaging and photodynamic (photothermal) therapy.

	**Chi-Kong Chung** Dr Arthur Chi-Kong Chung is a Research Assistant Professor in State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University since 2014. He received a B.S. from department of chemistry, the Chinese University of Hong Kong in 1989, and an M.S. from department of biology, the Chinese University of Hong Kong in 1992. He received his Ph.D. in Zoology from the University of Oklahoma, USA in 1998. From 1998 to 2006 he worked in Department of Molecular and Cellular Biology, Baylor College of Medicine, Houston, TX, USA as a post-doc and an instructor. His current interest about the effects of environmental organic pollutants on health diseases.
	**Yanjun Hong** Dr. Yanjun Hong is currently a Research Assistant Professor in State Key Laboratory of Environmental and Biological Analysis. She received her Bachelor's Degree in Pharmaceutical Science and Ph.D. in Pharmaceutical Analysis from Zhejiang University. Before joining HKBU in Aug. 2015, she did her Post-doc training in National University of Singapore. Her primary research interests are mass spectrometry-based metabolomics to: 1) study the toxicity of environmental pollutants; and 2) investigate the underlying pathogenesis mechanisms of human disease. Dr. Hong is also the principle investigator of several research grants funded by National Natural Science Foundation of China (NSFC) and Hong Kong Research Grants Council-General Research Fund (GRF).
	**Chao Zhao** Dr. Chao Zhao obtained her Ph.D. degree from the RCEES, CAS in prof. Hailin Wang's group. Later on she obtained the "Hong Kong Scholars Program" funding and pursued post-doc training in Prof. Zongwei Cai's group, and her research focus is multi-omics analysis, MS imaging and epigenetics.
	**Hongna Zhang** Dr. Hongna Zhang received Ph.D degree in 2017 in SKLECE, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences. Then she worked as a Post-Doctoral Fellow in SKLEBA, Hong Kong Baptist University. Her research interests are in the study of environmental process and the bioavailability of organic contaminants.

	**Hongzhi Zhao** Dr. Hongzhi Zhao is a post-doctor in the State Key Laboratory of Environmental and Biological Analysis. She got her bachelor's degree in Pharmaceutical Engineering and her master's degree in Biochemistry Engineering from Tianjin University. She has got her doctoral degree in Chemical Biology from College of Pharmacy, Nankai University. Her current research area is metabolomics and birth cohort.

Abstract

Formation and Fate of Unsaturated Aldehydes and Dicarbonyl Compounds During Oxidative Water Treatment

David Sedlak
University of California at Berkeley

It is well established that a variety of aldehydes are produced during oxidative water treatment (e.g., ozonation, advanced oxidation, in situ chemical oxidation). Although it is well known that these compounds have human health effects, they have not been considered as a major concern because most previous studies focused on a limited suite of saturated aldehydes that can be easily measured (e.g., formaldehyde, acetaldehyde). We have shown that, in addition to saturated aldehydes, oxidative treatment can lead to the formation of a suite of α,β-unsaturated carbonyl compounds. In particular, oxidation of alkyl-substituted aromatic compounds and phenolic compounds produce aldehydes and dicarbonyl compounds through direct ring cleavage in the early phase of advanced oxidation processes. To assess the potential transformation of these compounds during primary disinfection or in drinking water distribution systems, we measured rate constants and transformation products under a variety of conditions. For most compounds, apparent second-order rate constants for reactions with chlorine increased with increasing pH, and rate constants were linearly correlated with the fraction of HOCl as OCl-, implying that hypochlorite was the reactive species. Analysis of the intermediate products by NMR indicates that a variety of transformation products are formed, with many exhibiting structures that may be toxic. Overall, unsaturated aldehydes and carbonyls represent a class of compounds of concern whenever water undergoes oxidative treatment.

Fine Particles & Health Risk

Gui-bin Jiang

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China faces complex environmental pollution and health risk. The interaction between the epigenetic makeup of an individual and their environmental exposure record is accepted as a determinant factor for most human cancers. Pollution is the largest environmental cause of disease and premature death in the world today. It was demonstrated that air and water pollution is the major source of cancer morbidity & mortality. The haze in China has been become the most public concerned and challenging problem. The complexity of fine particulate matters (PM2.5) resulted in both high specificity and uncertainty of the toxic compositions and toxicity mechanisms. The Ambient PM mediated-Oxidative Stress and Genetic damage, Overwhelming of antioxidant and DNA repair mechanisms may result in oxidative stress and oxidative damage to DNA, lipids and proteins. There is strong evidence to support that airborne PM increases markers of genotoxicity: DNA adducts, cytogenetic damage, DNA strand breaks, oxidatively damaged DNA and gene mutation. This talk will focus on the Fine Particle Chemistry (FPC), defined as the study of chemical characterization, structure, nature, molecular transformation and toxicology of a fine particles, such as PM10, PM2.5, PM1.0, virus, bacterial, nanomaterials and so on.

Keywords: Fine Particle Chemistry, health risk

References

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Microfluidic Analytical System for Rapid Survey of Antimicrobial Resistance in Environmental Microorganisms

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Growing at alarming rate worldwide, antimicrobial resistance (AMR) is recognized as an imminent threat to global health and the modern society. Though much attention has been focused on the clinical use, the development of AMR in the environment, e.g., through non-therapeutic use of antibiotics in farming and improper discharge of drug-containing waste, is also calling for effective resolution. Accordingly, a cost-efficient portable system for routine survey in the environment is of demand. In recent years, reports proposed some new antimicrobial susceptibility testing (AST) methods based on microfluidics that takes only a few hours. Such new methods, however, haven't been translated into implementation mainly because of the requirement of expensive microscopes for observation and the issues of reliability caused by device fouling. In this work, we develop a microfluidic AST system that shows nice reliability and does not require microscope for observation. We demonstrate a reliable whole-PP microfluidic chip with 3D microchannels that shows several advantages compared to PDMS chips, including compatibility with multiple solvents and dyes, recyclability, low cost, as well as significantly less contamination. A "AST barcode" design is developed to allow direct observation of the results without using a microscope. It utilizes arrays of nano-filters which concentrate the cell density after the culturing step and generate barcodes that can be recorded and analyzed with a smart phone. In this way, layman can complete an AST survey from an environmental sample within half a day.

Application Example of Stem Cell Toxicology Model: Bisphenols Induced Development Neurotoxicity

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In recent years, the use of embryonic stem cells (ESCs) in toxicological applications has revolutionized the field. In this study, we investigated the overall toxicity of three typical environmental pollutants, Bisphenol A (BPA), Bisphenol F (BPF) and Bisphenol S (BPS), with an embryonic stem cell system. Our results indicate no obvious cytotoxic effects for the three chemicals on self-renewing ESCs, in the range of concentrations used (from 100 nM to 10 μM), as demonstrated by cell viability and oxidative stress measurements. However, BPA, BPF and BPS, showed significant potential developmental toxicity when we mimicked embryonic development in vitro by differentiating ESCs via embryoid body (EB) formation. In fact, we proved that BPA/BPF/BPS, after 20-day treatment, significantly impaired ectoderm specification, especially down-regulating neural ectoderm gene such as Pax6, Nestin, Sox1 and Sox3. The neurotoxic effects of BPA/BPF/BPS were also clearly implied in our two additional differentiation procedures specifically directed towards neural ectoderm and/or neural progenitor cells, via EB formation or in monolayer conditions. Contrary to the common understanding that BPA and its derivatives, BPF and BPS, cause toxicity by interfering with the estrogen receptor (ER) pathway, our Fulvestrant-based antagonistic experiments revealed the neurotoxic effects of the three chemicals were not related to the ER signaling cascade. Moreover, RNA-Seq analyses of BPA/BPF/BPS treated samples, harvested at different time points during the global, and neural progenitor cell-specific, EB-based differentiations, suggest multiple molecular mechanisms of toxicity, including disruption of the axon guidance and Wnt signaling pathways. Taken together, our study confirmed that BPA/BPF/BPS are developmental toxicants affecting gene expression during neural differentiation. We also demonstrated that our stem cell toxicology system could serve as a noteworthy improvement over traditional cell toxicity assays.

Preliminary Efficacy and Mechanism for Preventing and Treating Oral Leukoplakia Carcinogenesis by Ruthenium Complex with Tolfenamic Acid

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Oral leukoplakia is one of precancerous lesions, and has a high risk of development to oral squamous cell carcinoma (OSCC). It is a serious threat to human life and health. At present, the treatment for OSCC include surgery, drugs and laser. However, surgical treatment is easy to cause oral tissue defects. Drugs and laser treatment cannot effectively prevent the recurrence of oral leukoplakia. So the choice of safe and effective treatment methods has become the difficult subject. Photodynamic therapy (PDT) has the advantages of minimal invasiveness, small side effects and so on. It has been used to treat a variety of cancers, but rarely used in the prevention and treatment of oral leukoplakia. As a potential new group of PDT photosensitizer, Ru complexes in the presence of a suitable counteranion have been found to effectively enter the live-cell nucleus and induce apoptosis after light irradiation, and we expect that they can be used to prevent and treat oral leukoplakia. In the study, dysplastic oral keratinocytes (DOK cell), the cell line of oral precancerous lesions was selected and 5-amino-laviolinic acid (ALA) was used as a positive control. We found that after [Ru(bpy)2dppz]2+/Tolfenamic acid (Ru/TA) intervention and light exposure, the proliferation of DOK cells was inhibited and singlet oxygen was produced. Ru/TA can play the role of photosensitizer. Further verified on the oral squamous cell line CAL27 and oral mucosal fibroblasts, we found that Ru/TA can enter the nucleus, induce the apoptosis of DOK and Cal 27 cells, and can accumulate reactive oxygen in cells to produce phototoxic effects. DMBA was then used to induce the establishment of an oral leukoplakia animal model on the golden hamster. After Ru/TA treatment, the fluorescent effect can be detected in the lesions of oral leukoplakia with small animal living imager. The clinical and pathological changes of oral leukoplakia were observed after one week, two weeks and six months of PDT. And the efficacy was evaluated. The results indicated that Ru/TA treatment can inhibit the proliferation and carcinogenesis of oral mucosal epithelium, make oral leukoplakia recede, and achieve the effect of prevention and treatment for oral leukoplakia.

References

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DTT Activity and ROS Generation Ability of Water-Soluble PM2.5 in Hong Kong: Characterization and Source Apportionment

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A comprehensive characterization and source apportionment of oxidative potential (OP) induced by water-soluble PM2.5 collected in Hong Kong during a one-year period were conducted. Reactive oxygen species (ROS) generation ability of water-soluble PM2.5 was assessed in terms of dithiothreitol (DTT) consumption and ·OH formation using a DTT assay. No correlation was observed between measured DTT consumption and ·OH generation, and both of them showed high values on days mainly influenced by regional pollution sources, indicating more ROS active PM2.5 components generated or transported to Hong Kong under this condition. Sampled air volume-normalized DTT activity (DTTV) and ·OH generation (·OHV), together with various chemical source markers, were then input into positive matrix factorization (PMF), and six sources of water-soluble PM2.5 associated OP were apportioned, i.e. secondary sulfate, biomass burning, secondary organic aerosol (SOA), vehicle emissions, marine vessels and metal factor. Primary sources accounted for 83.5% of DTTV, with metal factor as the leading contributor on days under regional and long regional transport pollution, and marine vessels to be the most significant on the days under local pollution. Metal factor also made the predominant contribution (84.5%) to ·OH generation throughout the year. All six sources were found to be DTT active, however, only three sources, i.e. metal factor, vehicle emissions, and SOA, showed contributions to ·OH generation. Based on PMF results, we further evaluate the intrinsic ROS generation ability of water soluble PM2.5 from each source. Marine vessels exhibited the highest intrinsic DTT activity (0.174 nmol min-1 μg-1 PM2.5); while metal factor was the most effective source in ·OH generation (0.106 pmol min-1 μg-1 PM2.5).

Arsenic Adsorptive Removal Using TiO_2 And Beyond

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State Key Laboratory of Environmental Chemistry and Ecotoxicology, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing, China

Arsenic is a carcinogen in groundwater in many places worldwide. Adsorption on TiO2 nanomaterials provides a promising technique for arsenic removal. Though the adsorption mechanism is well known to involve the formation of a bidentate binuclear surface complex, even TiO2 of the same anatase phase from different sources exhibit distinct adsorption and photo-catalytic capacities. The lack of conformity of many experimental observations with the general belief that particle size or surface area regulates TiO2 adsorption motivates our study.

Our results from multiple complementary characterization techniques suggest that anatase {001} facets have stronger Lewis acid sites than those on {101} facets, resulting in a higher As adsorption affinity. Density functional theory (DFT) calculations confirmed that the As surface complex is more energetically favorable on {001} than on {101} facets. In addition, the redox transformation and fate of adsorbed arsenic on TiO2 were explored in the presence of indigenous bacteria strains. The insights gained from this study provide a firm basis for the proposition that As adsorption can be mediated by tailoring the exposed TiO2 facets.

Exposure to BDE-47 Promotes Obesity and Aggravates Liver Dysfunction in Diet-Induced Obesity Mice

Arthur C.K. Chung
State Key Laboratory of Environmental and Biological Analysis, Department of Chemistry, Hong Kong Baptist University, Hong Kong, China;

Exposure to persistent organic pollutants (POPs), has been associated with obesity. However, their lipid toxicities and detailed mechanism related to obesity is unknown. We employed diet-induced mouse model to examine obesogenic effects of 2, 2', 4, 4'-tetra-brominated biphenyl ether (BDE 47) and the cell model to determine the mechanism of BDE 47 on obesity. BDE-47 exposure (70mg/kg) to mice with high fat diet (HED) significantly promoted the elevation of body weight gain and body size. Liver histology and increased triglyceride content showed that the exposure of BDE-47 in HFD group worsened hepatic steatosis, accompanied with increased inflammation, compared to controls. Results from lipidomics and expression analyses revealed that BDE-47 up-regulated triglyceride synthesis but suppressed β oxidation and triglyceride exportation, which might lead to the accumulation of hepatic lipid in mice with HFD. In addition, BDE 47 exposure (5 or 10 μM) also promoted adipocyte differentiation by enhancing lipid accumulation and expression levels of biomarkers of adipogenesis. BDE 47 also upregulated purine metabolism and altered glutathione metabolism to promote oxidative stress and uric acid production in adipocytes. Antioxidant treatments, including the suppression of xanthine oxidase, inhibited the obesogenic effects of BDE 47 on inducing oxidative stress and lipid accumulation. In conclusion, BDE 47 is potential environmental obesogen by which providing a permissive oxidative environment for inducing adipocyte differentiation. Our results provide new evidence that exposure to environmental organic pollutant play a pathological role in in diet-induced obesity and related liver dysfunction.

Profiling of DNA Modifications for Environmental Epigenetics

Hailin Wang
State Key Laboratory of Environmental Chemistry and Ecotoxicology, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing, China

Genetic DNA molecules take four bases (adenine, thymine, cytosine, guanine) exclusively to code heritable information in all the three domains of life. Adding, deleting, and substituting any of these bases in the context of genomic sequences would permanently change the genetic information. Endogenous and/or exogenous stresses may cause potent insults on genomes to form DNA damages through reactive oxygen/nitrogen/carbon species or substitution. These damages to DNA bases will cause persistent changes during DNA replication if they are not correctly repaired or bypassed, leading to heritable mutations. Interestingly, there are a few modifications enzymatically set on cytosine, which regulates gene expression and chromosome structures without changing the hereditary sequences. These DNA modifications are usually attributed to epigenetic markers. The known epigenetic cytosine modifications of mammals include 5-methyl-20-deoxycytidine (5mdC) and its oxidized derivatives 5-(hydroxymethyl)-2'-deoxycytidine (5hmdC), 5-formyl-2'--deoxycytidine (5fdC) and 5-carboxy-2'-deoxycytidine (5cadC) . We discovered N6-methyl-20-deoxyadenosine (6mdA) as a new DNA modification in Drosophila Meloganster, and Greer et al. showed the presence of thismodification in Caenorhabditis elegans. Together with the genome-wide 6mdA sequencing of Chlamydomonas, these studies proposed that it is a potential epigenetic marker in eukaryotes. An intriguing base is 5-hydroxymethyluridine, which could be formed by oxidation of thymine (in DNA) as catalyzed by Tet dioxygenases or deamination of 5-hydroxymethylcytosine (in DNA) as catalyzed by AID/APOBEC family proteins, and also by Fenton reactions. However, the deamination of 5-hydroxymethylcytosine in genome is not supported with structural analysis of AID/APOBEC deaminases-DNA complexes, and thus it remains elusive. Among this base modified-nucleosides, 5hmdC, 5fdC and 5-(hydroxymethyl)-20-deoxyuridine (5hmdU) are not only formed by the catalytic action of Tet dioxygenases as epigenetic modifications, and also generated (but at much less probability) as the products of radical reactions.

In addition to fundamental research on DNA modifications (not described here), we also focused on the interaction of environmental molecules with epigenetic DNA modifications, including vitamin C, redox quinones, heavy metals and drugs. Here we took heavy metal nickel as an example. Nickel is one of heavy metals found widely in

the environment. It is an essential microelement but also toxic. However, nickel displays only weak genotoxicity and mutagenicity. Exploration of the epigenetic toxicity of nickel is extremely interesting. By the use of UHPLC-MS/MS for detection of 5hmdC, we found that Ni(II) dramatically inhibits Tet proteins mediated oxidation of DNA 5mdC in vitro, and in cells ranging from somatic cell lines to embryonic stem cells, as manifested by the consistent observation of a significant decrease in 5hmdC. We further used a size exclusion chromatography (SEC)einductively coupled plasmaemass spectrometry (ICP-MS) method to measure Tet proteineNi(II) binding events. By the use of SEC, the biomolecules diffuse according to size when moving along with mobile phase because the pores of different sizes are widely distributed along with the stationary particles. Essentially, the molecules of larger sizes can access few pores of large size, showing shorter retention times; on the other hand, molecules of smaller sizes will access more pores from smaller sizes to large sizes, showing longer retention times. By this mechanism, the Tet protein-bound Ni(II) can be well separated from unbound (free) Ni(II). Moreover, ICP-MS can be used for selective detection of Ni(II). It found that natural Ni(II) ion can bind to the Fe(II)-chelating motif (HXD, H1382, D1384, H1881, and H1416) and replace Fe(II). This is reasonable that Ni(II) is highly similar to Fe(II) in terms of charge and ionic radius (Fe(II), 0.061 nm; Ni(II), 0.069 nm). Unexpectedly, Ni(II) has an affinity of 7.5-fold as high as Fe(II). Consistently, we further found that Ni(II) ion inhibits Tet-mediated 5mdC oxidation activity with an estimated IC50 of 1.2 mM. Essentially, Ni(II) can be used as a high affinity and selective inhibitor to explore the function and dynamics of Tet proteins. Of note, the well-known inhibitors are an oncometabolite 2-hydroxyglutarate (2-HG) and a synthetic dimethyloxalylglycine (DMOG), but they may displace the cofactor a-ketoglutarate from the catalytic center at the concentrations of mM.

Separation and Determination of Trace Nanoparticles in Complex Matrices

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Nanoparticles (NPs) are present in the environment due to their natural formation and the wide application of engineered NPs. To understand their occurrence, distribution, transport, fate, effects and biosafety, it is of great importance to develop methods for efficient and sensitive determination of NPs in complex matrices like environmental and biological samples. As the composition, structure, species and size of NPs have remarkable impacts on their environmental processes and biological effects, it is necessary to determine their composition and concentration, as well as to characterize their size, shape and surface charge. We have developed various methods for analysis of NPs in the environmental and biological samples. Cloud point extraction (CPE) and membrane-based solid phase extraction (SPE) were applied to selectively separate various NPs from the matrices. Size fractionation techniques, such as size-exclusion chromatography and field flow fractionation (FFF), were combined with inductively coupled plasma mass spectrometry (ICP-MS) for identification, mass quantification and size characterization of NPs. These above methods were applied to trace the transformation of NPs in the environment and organisms.

Effects of PFOS on the Gut Microbiome and Metabolic Profiles in Mice

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Perfluorooctane sulfonate (PFOS) is a persistent organic pollutant that has been detected almost ubiquitously in environmental media and biological samples. Liver has been demonstrated to be the main target organ of PFOS. With the growing recognition of the importance of liver-gut microbiota axis, it is possible that gut microbiota perturbation may also contribute to PFOS-induced liver toxicity. In this study, we investigated the effects of PFOS on the gut microbiome and its metabolic profiles in CD-1 mice, using 16S rRNA gene sequencing and mass spectrometry-based metabolomics. Steatosis and inflammatory cell infiltration were observed in the liver of the exposure group. PFOS significantly perturbed the gut microbiome composition in a sex-specific manner. Bacteria species including *Lactobacillus_Reuteri* and *Lactobacillus_vaginalis* were only significantly perturbed in male mice with PFOS exposure, while *Akkermansia_Muciniphila* and *Bifidobacterium_Pseudolongum* were only changed in female mice. Clear separations of metabolic profiles between control and PFOS-treated groups were observed in fecal samples for both male and female mice. Interestingly, the main metabolites that contribute to group discrimination are related to amino acid metabolism in a sex-dependent manner. The perturbations of the gut microbiome and its metabolic profiles may serve as a new mechanism of liver toxicity induced by PFOS. Further studies including antibiotic treatment, fecal microbiota transplant and bacterial treatment will be performed to validate the relationship between the perturbed bacteria species, metabolic profiles, and the liver injury.

FASs Exposure Relates to Oxidative Stress, Fatty Acid β-Oxidation Disorder, and Potential Kidney Injury in Occupational Workers in a Manufactory in China

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Occupational workers are usually exposed to high levels of per-and polyfluoroalkyl substances (PFASs), which makes them under greater health risks compared to the general population. In this study, mass spectrometry-based metabolomics was used to investigate the potential health risks of occupational PFASs exposure to workers in a manufactory in China. 40 occupational workers and 52 control subjects from the general population were involved. The PFAS levels in plasma from both groups were analyzed. Six PFAS congeners (∑6PFASs) were found to be main components of the 13 detected PFASs, with a geometric mean of 1770 and 22.2 ng mL-1 in occupational workers and the general population, respectively. Metabolic profiles of the plasma samples were acquired using liquid chromatography coupled with orbitrap high-resolution mass spectrometry and gas chromatography-mass spectrometry. The partial least squares-discriminant analysis model indicated that the metabolic profiles in the plasma of two groups could be clearly separated. Fourteen potential biomarkers between the two groups were identified and they were found to be correlated with oxidative stress, fatty acid β-oxidation, and potential kidney injury. The obtained results indicated that the health effects of the high PFASs exposure level on occupational workers should not be ignored.

Porphyrin-Implanted Carbon Nanodots for Photoacoustic Imaging and in Vivo Breast Cancer Ablation

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The incorporation of intensive light absorbing porphyrins macrocycles with biocompatible nanoparticles would lead to new nanomaterials with multiple imaging and therapeutic modalities. Herein, a facile synthetic strategy has been applied to prepare porphyrin-implanted carbon nanodots (PNDs) by partial and selective pyrolysis of 5,10,15,20-tetrakis(4-aminophenyl)porphyrin (TAPP) and citric acid (CA) at an appropriate temperature. As-prepared PNDs exhibit not only the excellent stability and biocompatibility characteristic of carbon nanodots but also the unique properties of porphyrin macrocycle such as strong UV−visible and near-infrared absorption, specifically, high photodynamic therapy efficiency. More importantly, the PNDs with near-infrared absorption could act as a contrast agent for photoacoustic molecular imaging with deep tissue penetration and fine spatial resolution. The Cetuximab-conjugated porphyrin-based carbon nanodots (C225-PNDs) have been further prepared to precisely target the cancer cells (HCC827 and MDA-MB-231 cells) with overexpression of EGFR, leading to highly efficient photodynamic therapy upon two-photo excitation at 800 nm. A complete ablation of tumor together with an enhanced photoacoustic contrast ability for C225-PNDs have been further validated in mice bearing MDA-MB-231 breast cancer.

Seasonal Variation and Human Exposure Assessment of Legacy And Novel Brominated Flame Retardants in PM2.5 in Different Microenvironments in Beijing, China

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Indoor exposure to legacy and novel brominated flame retardants (NBFRs) may cause potential risks to human health. We investigated the seasonal variations of PM2.5-bound polybrominated diphenyl ethers (PBDEs) and NBFRs in various indoor environments (i.e. activity room, dormitory, home and office) and outdoor PM2.5 in Beijing, China over one year. PBDE levels (226 ± 108 pg m-3) were higher than that of NBFRs (27.0 ± 16.0 pg m-3) in all indoor environments. Decabromodiphenyl ether (BDE-209) and decabromodiphenyl ethane (DBDPE) were the most abundant BFRs. Office showed the highest mean concentrations of Σ15PBDEs (251 ± 125 pg m-3) and Σ9NBFRs (33.0 ± 18.0 pg m-3), which may be related to the higher number density of indoor materials. The concentrations of Σ9NBFRs and Σ15PBDE in indoor PM2.5 were found to be significantly higher than those in the corresponding outdoor PM2.5 ($p < 0.05$). Two to twenty-fold seasonal variation was observed for levels of PM2.5-bound BFRs during one year, and the indoor concentration increased slightly during the central-heating period. The PM2.5-bound BFRs concentrations in PM2.5 were significantly negatively correlated with temperature and relative humidity, while positively correlated with in PM2.5 concentrations ($p < 0.05$). Atmosphere haze pollution could possibly contribute to higher levels of indoor PM2.5-bound BFRs. Human daily intake of BFRs via PM2.5 inhalation showed seasonal differences, which the highest exposure risk occurred in winter. Toddlers were assessed to be more vulnerable to indoor PM2.5-bound BFRs in all seasons. Our study provided the first-hand measurements of seasonal concentrations and human exposure of PM2.5-bound BFRs in different indoor scenarios in Beijing.

Silver Nanoparticles Impair Generation of Amputated Zebrafish Fins

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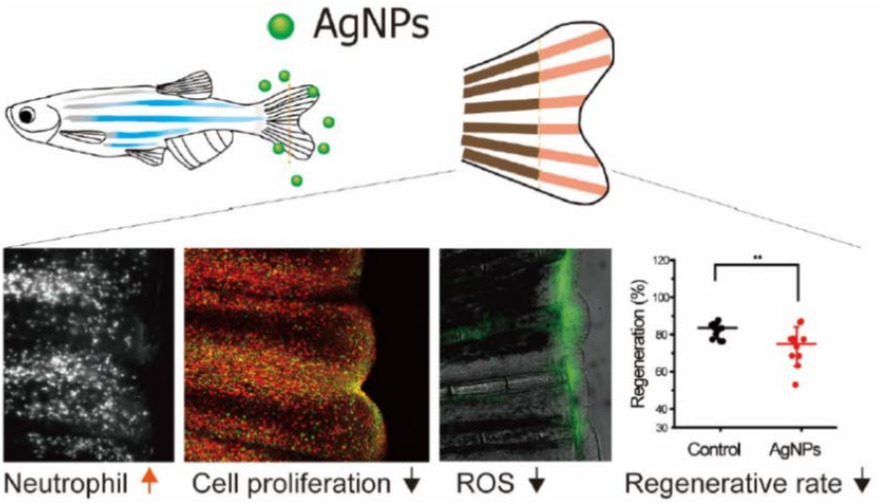
Dressings coated with silver nanoparticles (AgNPs) have been widely used in the clinical therapy of dermal wounds due to their beneficial effects on controlling wound infection. However, in vivo studies regarding the toxic effects of AgNPs on wound healing are limited, and the conclusions remain controversial. In our study, the regeneration of amputated zebrafish fins was used as an in vivo model to evaluate the effects of AgNPs on wound healing. We demonstrated that AgNPs treatment impaired fin regeneration in an exposure stage-dependent manner, and the phase of epithelialization and the beginning of blastemal formation were the most sensitive stage to AgNPs toxicity. Moreover, nanoparticles, but not the released ions (Ag+) exerted the toxic effects. Further studies showed that theinflammatory response of neutrophils was slightly increased after AgNPs exposure. Additionally, AgNPs treatment resulted in a decrease in the cell proliferation of the regenerative blastemal and in the amputation-induced generation of reactive oxygen species. Our studies provide evidence that AgNPs obstruct tissue regeneration in dermal wounds, suggesting that the potential adverse effects of AgNPs-coated dressings should be taken into consideration during wound care.



Develop Small Analytical Equipment and Devices Using 3D Printing Technology

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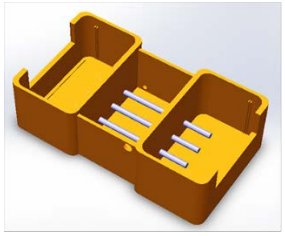
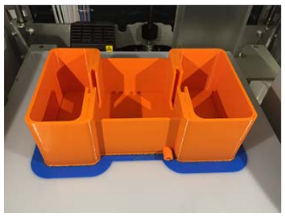
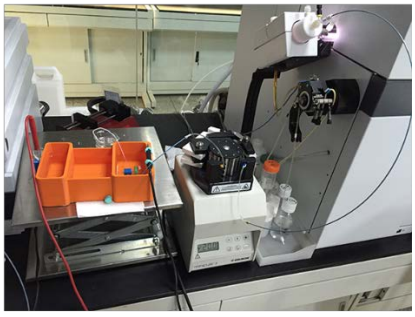
3D printing technology has been rapidly developed in recent years. The outstanding ability of 3D printing to build customized, personalized and complex-structured devices has made it widely applied in many fields including machining, architecture, aerospace, biotechnology, medicine, electronic engineering and so on. However, the application of 3D printing in chemistry is still limited. Recently, we have developed a variety of small analytical devices with 3D printing technology in our laboratory, such as a GE-ICP MS system used for online separation and detection of metalloproteins, a “matrix free” target for MALDI-TOF-MS permitting direct analysis of small molecular samples and a single-pass spray chamber for ICP MS. These applications not only show the convenience and accuracy of 3D printing technology in the replication and reconstruction of existing analysis devices, but also demonstrate that further optimization and improvement can be easily realized with 3D printing technology. Furthermore, the innovation of 3D printable materials will make a qualitative leap in the performance of original devices. The further development of 3D printing technology in analytical technology and equipment development will definitely bring revolutionary breakthroughs to this field.







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Airborne Fine Particulate Matter Induces Cognitive and Emotional Disorders in Offspring Mice Exposed During Pregnancy

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Gestational exposure to airborne fine particulate matter with size of < 2.5 μm ($PM_{2.5}$) is associated with adverse postnatal outcomes. Placenta-fetus-offspring in mice were investigated using a comprehensive approach including mass spectrometry-based lipidomics and three-dimensional mass spectrometry imaging technology. Our results demonstrated that gestational exposure to $PM_{2.5}$ showed cognitive and emotional disorders in female offspring despite these offspring having never been exposed to $PM_{2.5}$. We further found that $PM_{2.5}$ exposure induced impairment of placental cytoarchitecture, increase of neuro-degeneration in hippocampus and significant lipidome reprogramming, which may affect the modulation of maternal-fetal cross-talk and result in the behavior disorders.

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Integration of Metabolomics and Lipidomics Reveals Metabolic Mechanisms of Triclosan-Induced Toxicity in Human Hepatocytes

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Triclosan (TCS), an extensively used antimicrobial agent, has raised considerable concern due to its hepatocarcinogenic potential. However, previous hepatotoxicity studies primarily focused on the activation of specific intracellular receptors, the underlying mechanisms still warrant further investigation at the metabolic level. Herein, we applied metabolomics in combination with lipidomics to unveil TCS-related metabolic responses in human normal and cancerous hepatocytes. Endogenous and exogenous metabolites were analyzed for the identification of metabolic biomarkers and biotransformation products. In L02 normal cells, TCS exposure induced the up-regulation of purine metabolism and amino acid metabolism, caused lipid accumulation and disturbed energy metabolism. These metabolic disorders in turn enhanced the overproduction of reactive oxygen species (ROS), leading to the alteration of antioxidant enzyme activities, down-regulation of endogenous antioxidants and peroxidation of lipids. TCS-induced oxidative stress is thus considered to be one crucial factor for hepatotoxicity. However, in HepG2 cancer cells, TCS underwent fast detoxification through phase II metabolism, accompanied by the enhancement of energy metabolism and elevation of antioxidant defense system, which contributed to the potential effects of TCS on human hepatocellular carcinoma development. These different responses of metabolism between normal and cancerous hepatocytes provide novel and robust perspectives for revealing the mechanisms of TCS-triggered hepatotoxicity.

Toxicity of Black Phosphorus Nanosheets

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Black phosphorus nanosheets (BPs) is a layered semiconductor that consists of corrugated planes of phosphorus atoms with strong intralayer bonding and weak interlayer interactions. Few-layer BPs has a thickness-tunable bandgap, As the promising characteristics, BPs is becoming a powerful agent for various biomedical applications. However, their biocompatibility thus warrants a detailed evaluation of the safety for BPs use. Although immune system plays a protective role in the defense against infected microbial pathogens in the body, it is also responsible for the clearance of nanomaterials from the circulation. Some nanomaterials display several types of adverse effect upon injected into mice, which could then damage normal tissues.
In the current study, we investigated the toxicity of BPs. Biological effects of BPs with and without titanium sulfonate ligand (TiL4) modification are investigated. We firstly evaluated the cytotoxicity of BPs using macrophages as cell model. We found BPs displayed high potential to be engulfed by macrophages. The intracellular BPs triggered significant cell death. Comparing with control cells, BPs exposure also resulted in the generation of various proinflammatory cytokines. In contrast, In vitro experiments suggest that TiL4 modification can reduce the uptake by macrophages, and further attenuate the cytotoxicity and proinflammation. Our results suggested that the side effect of BPs needed to be evaluated in detail when applied in therapeutics in the future.The detailed investigation of biological effects of BPs may guide their applications as foreign particles administered to animals or humans.

The Health Risk of Environmental Pollutants Exposure and Metabolomics Study on Pregnant Disease

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Extensive studies have shown that prenatal exposure to environmental pollutants might have a variety of adverse health effects on both pregnant women and offspring. However, the health risk of environmental pollutants and the development of pregnant disease are still not fully understood. Thus, a project based on a birth cohort was undertaken with the objectives of investigating the health risk of environmental pollutants exposure and obtaining a better understanding of the potential pathogenesis of diseases during pregnancy.

This project included three parts. Firstly, screening of the exposure of environmental pollutants to pregnant women was performed. The methods for the determination eight categories of pollutants including nine organochlorine pesticides, nine bisphenols, nine phthalates, six benzophenones, five parabens, five benzothiazoles, six benzotriazoles, three other phenols, were developed by using ultra-high performance liquid chromatography (or gas chromatography) coupled with triple quadrupole mass spectrometry. The prenatal exposures to the environmental pollutants were evaluated through maternal urine or cord blood samples. Secondly, the association of pollutants exposure and health outcomes of pregnant women and offspring was investigated. We found that prenatal exposure of β-hexachlorocyclohexane was negatively associated with birth weight in female offspring, while prenatal exposure to the pollutants such as triclosan and benzophenone may be associated with blood pressure. Thirdly, metabolomics approach was applied for the study on gestational diabetes mellitus, the most common disease during pregnancy. Metabolites in amino acid metabolism, purine metabolism and other pathways were found to be altered prior to gestational diabetes mellitus onset and may play a role in its pathogenesis.

The findings of this project may provide information to the study on health effects of environmental pollutants and may have important public health implications.

Molecular Fractionation of DOM on Iron Oxyhydroxides

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Interactions between dissolved organic matter (DOM) and iron oxyhydroxides have important environmental and geochemical implications. Here, we investigated the interfacial behaviour of DOM on different iron oxyhydroxides using electrospray ionization coupled with Fourier-transform ion cyclotron resonance mass spectrometry (ESI-FT-ICR-MS). Firstly, we found that adsorption on iron oxyhydroxides induced molecular fractionation of DOM at water-solid interface, and ferrihydrite induced more pronounced molecular fractionation of DOM than other iron oxyhydroxides. Molecules with high molecular weight (>500 Da), high oxidation state or high in unsaturation such as oxidized black carbon, polyphenol- and tannic-like compounds had higher affinity to iron oxyhydroxides, while compounds like carbohydrates and aliphatics were preferentially maintained in solution. Furthermore, we investigated the molecular mechanism of iron oxyhydroxides induced molecular fractionation of DOM. Two hematite nanocrystals with well-controlled crystalline architectures were used as models. Result indicated that hematite with a predominant exposure of {100} facets induced more pronounced adsorption and molecular fractionation of DOM than {001} facets, indicating that the interfacial adsorptive fractionation process of DOM was mediated by exposed facets of hematite. Further exploration of the surface hydroxyl groups of the two hematite nanocrystals confirmed that the facet-mediated molecular fractionation of DOM was attributable to the abundance of singly iron-atom coordinated -OH sites (-FeOH) on the hematite surfaces. It was the ligand-exchange between special DOM molecules and singly-coordinated -OH groups on the hematite surfaces induced the selective binding and molecular fractionation of DOM at the mineral-water interface. This -FeOH dependent molecular fractionation mechanism can also explain the adsorptive fractionation of DOM on other iron oxyhydroxides. The above results contribute to our understanding of the molecular exchanges of DOM at water-soil or sediment interface.

Molecular Characterization of Natural Organic Matter by ESI-Fourier Transform Ion Cyclotron Resonance Mass Spectrometry

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Natural organic matter (NOM) is a complex organic mixture and plays a crucial role in environmental processes. By using Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS), detailed molecular information of NOM could be achieved. In this paper, ion accumulation time (IAT), a key parameter of FTICR-MS for complex mixture detection, was focused on, and its effect on the molecular characterization of NOM by FTICR-MS was systematically investigated. A notable feature of selective detection of NOM molecules by FTICR-MS with different IAT was observed. Most of polar molecules with high O/C ratio (O/C ratio>0.5) could be easily detected by FTICR-MS with a short IAT, but extending IAT leaded to the ion intensities of these molecules decreasing or even disappearing. Meanwhile, a large number of unsaturated and aromatic molecules with low O/C ratio (O/C ratio<0.6) and low polarity, all of which could not be observed with a short IAT, were remarkably detected by extending IAT. Results also revealed that the unsaturated and aromatic molecules, which could only be observed by extending IAT, were not generated by the fragmentation of molecules in NOM or from the dissociation of NOM aggregations but originally existed in NOM samples. The selective detection of NOM molecules caused by IAT extending was possibly attributed to their different polarity and different stability in the collision cell. Based on these results, a novel strategy of combination of mass spectrometric data of NOM obtained with different IAT by FTICR-MS was proposed. By this strategy, more than 4715 CHO-molecular formulas were assigned, where about 2000 more formulas were obtained in comparison with using a short IAT (2733 CHO-molecular formulas identified) solely. The strategy is simple and robust, and could be used as an alternative method to obtain more molecular information of NOM in the environment.

Non-Targeted Screening of Organic Pollutants in the Atmosphere by FT-ICR MS and GC×GC-HR TOF MS

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Several epidemiological studies have demonstrated the relevance of ambient particles in health effect. The traditional analysis for organics in PM2.5 is based on the targeted compounds, making it insufficient to explain much of the association between ambient particulate matter and health outcomes. Due to severe chromatographic interference and difficulty in identifying unknown structures, it is still a great challenge to understand the complex chemical components in the atmosphere. In this study, a systematic non-targeted analysis workflow using FT-ICR MS and GC×GC–HRTOFMS was developed, which enable us to conduct high-throughput screening of organics and more confidently identify the unknowns. Gas phase and different particle size samples in Beijing were collected and analyzed. The molecular element composition of more than 8000 organic compounds was obtained by FT-ICR MS, and CHO was found to be the main group. These compounds were then analyzed with KMD, RDBE vs Carbon Number and Van Krevelen three molecular characterization methods. And they were mainly composed of highly unsaturated, phenolic and fatty substances. The separation of thousands of compounds in one injection was achieved via the optimization of a series of parameters within GC×GC–HRTOFMS. It was found that more semi-volatile organic pollutants were distributed on the particles with particle size less than 1.0 μm. A variety of alkanes, olefins, aldehydes, ketones, acids, esters and aromatic compounds were rapidly screened by writing ion filtration program. Compounds that have the same parent structure and differ by the number of substituent groups were filtered via Mass Defect analysis. Tentative identification of some other unknown compounds was aided by library searching and structure diagnostic fragmentation combined with accurate mass and isotope information. The physical and chemical properties and toxicity of newly discovered substances would be predicted using the QSAR model. Therefore, comprehensive analysis and chemical characterization of organic pollutants in the atmosphere was acquired, which can contribute to understand the formation process, control measures, and health hazard of atmospheric pollution.