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CHEMICAL EFFECTS

Exposure concentration ratios and biological responses play a critical role in determining the joint toxicity of TiO₂ nanoparticles and As(V) to the organism: The case study in marine algae *Phaeodactylum tricornutum*

2023-11-16

Environmental risks of manufactured nanomaterials (MNMs) have been widely investigated while the understanding for joint toxicity mechanism of MNMs with other contaminants is still limited. This limitation may be attributed to variations in the concentration ratios of MNMs and co-existing contaminants in the real environment. To better assess the joint toxicity and clarify its underlying mechanisms, this study exposed *Phaeodactylum tricornutum* to different concentration combinations of nano-sized titanium dioxide (nTiO₂) and As(V) at toxic unit (TU) ratios of 1:4, 1:1, and 4:1. The results demonstrated that the joint toxicity modes of nTiO₂ and As(V) varied with the TU ratios exhibiting synergism for 1:4, partially addition for 1:1, and antagonism for 4:1. Specifically, at low TU ratio of 1:4, the adsorption of As(V) by nTiO₂ together with the subsequent internalization of nTiO₂ promoted a significant enrichment of As in algae. Simultaneously, the up-regulation of *pst* (phosphate transporter) genes in charge of the As(V) transport molecular further exacerbated the enrichment of inorganic As in algae, while the down-regulation of *ArsM* (arsenite S-adenosylmethionine methyltransferases) genes in charge of the As metabolism inhibited As biotransformation from toxic inorganic to nontoxic organic, causing the aggravated accumulation of toxic inorganic As in algae. At higher TU ratios of 1:1 and 4:1, the accumulation of As decreased in algae due to the higher sedimentation of nTiO₂ and thus the lower internalization of As-adsorbed nTiO₂, as well as the down-regulation of *pst* genes restricting the transportation of As(V) into algal cells, which jointly accelerated the As biotransformation from toxic inorganic to nontoxic organic. Our results suggest that more attention should be paid to exposure concentration ratios of MNMs and co-existing contaminants and biological responses including bioavailability, bioaccumulation, biotransformation, which would play a critical role in determining the joint toxicity to the organism.

Authors: Wei Qian, Ciara Chun Chen, Yuxiong Huang, Xiaoshan Zhu

Full Source: The Science of the total environment 2023 Nov 16:909:168508. doi: 10.1016/j.scitotenv.2023.168508.

Environmental risks of manufactured nanomaterials (MNMs) have been widely investigated while the understanding for joint toxicity mechanism of MNMs with other contaminants is still limited.

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Spatial heterogeneity and compositional profiles of dissolved organic matter in farmland soils across mainland China

2024-03

Dissolved organic matter (DOM) plays an essential role in many geochemical processes, however its complexity, chemical diversity, and molecular composition are poorly understood. Soil samples were collected from 500 vegetable fields in administrative regions of mainland China, of which 122 were selected for further investigation. DOM properties were characterized by three-dimensional excitation-emission matrix (3D-EEM) fluorescence spectroscopy and Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS) (field intensity is 15 Tesla). Our results indicated that the main constituents were UVA humic-like substances, humic-like substances, fulvic acid-like substances, and tyrosine-like substances. A total of 10,989 molecular formulae with a mass range of 100.04 to 799.59 Da were detected, covering the mass spectrometric information of the soil samples from 27 different regions. CHO and CHON molecules were dominant in DOM, whereas lignin, tannins, and aromatic substances served as the main components. The results of cluster analysis revealed that the soil properties in Jiangxi Province were considerably different from those in other regions. The key backgrounds of the DOM molecular characteristics in the vegetable-field soil samples across mainland China were provided at the molecular level, with large abundance and great variability.

Authors: Bingjun Han, Liyuan Chen, Kang Xiao, Yang Liu, Dong Cao, Lu Yu, Yujun Li, Shu Tao, Wenxin Liu

Full Source: Journal of environmental sciences (China) 2024 Mar:137:593-603. doi: 10.1016/j.jes.2023.02.042.

Dissolved organic matter (DOM) plays an essential role in many geochemical processes, however its complexity, chemical diversity, and molecular composition are poorly understood.

ENVIRONMENTAL RESEARCH

Photodegradation of biodegradable plastics in aquatic environments: Current understanding and challenges

2023-11-17

Direct photolysis and indirect photolysis are important abiotic processes in aquatic environments through which plastics can be transformed physically and chemically. Transport of biodegradable plastics in water is influenced by vertical mixing and turbulent flow, which make biodegradable plastics remain susceptible to sunlight and photolysis despite their high density. In general, biodegradable plastics are composed of ester containing polymers (e.g., poly(butylene succinate),

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polyhydroxyalkanoate, and polylactic acid), whereas non-biodegradable plastics are composed of long chains of saturated aliphatic hydrocarbons in their backbones (e.g., polyethylene, polypropylene, and polystyrene). Based on the reviewed knowledge and discussion, we may hypothesize that 1) direct photolysis is more pronounced for non-biodegradation than for biodegradable plastics, 2) smaller plastics such as micro/nanoplastics are more prone to photodegradation and photo-transformation by direct and indirect photolysis, 3) the production rate of reactive oxygen species (ROS) on the surface of biodegradable plastics is higher than that of non-biodegradable plastics, 4) the photodegradation of biodegradable plastics may be promoted by ROS produced from biodegradable plastics themselves, and 5) the subsequent reactions of ROS are more active on biodegradable plastics than non-biodegradable plastics. Moreover, micro/nanoplastics derived from biodegradable plastics serve as more effective carriers of organic pollutants than those from non-biodegradable plastics and thus biodegradable plastics may not necessarily be more ecofriendly than non-biodegradable plastics. However, biodegradable plastics have been largely unexplored from the viewpoint of direct or indirect photolysis. Roles of reactive oxygen species originating from biodegradable plastics should be further explored for comprehensively understanding the photodegradation of biodegradable plastics.

Authors: Vinhteang Kaing, Zhongyu Guo, Ty Sok, Dilini Kodikara, Florian Breider, Chihiro Yoshimura

Full Source: The Science of the total environment 2023 Nov 17:168539. doi: 10.1016/j.scitotenv.2023.168539.

Nano-size cobalt-doped cerium oxide particles embedded into graphitic carbon nitride for enhanced electrochemical sensing of insecticide fenitrothion in environmental samples: An experimental study with the theoretical elucidation of redox events

2023-11-15

In the present work, a nanocomposite, based on embedding Co-doped CeO₂ nanoparticles into graphitic carbon nitride (g-C₃N₄), was applied to functionalize commercial glassy carbon paste. This is the first application of the electrochemical sensor, developed through the proposed procedure, in electrochemical sensing. The sensor was utilized for the electrochemical determination of organophosphate pesticide fenitrothion (FNT). Cyclic voltammetry identified reversible oxidation of FNT (oxidation at 0.18 V and reduction at 0.13 V) and additional reduction at -0.62 V vs.

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Ag/AgCl in HCl solution (pH = 1). Theoretical calculations were carried out to model and elucidate experimentally observed redox processes. Special attention was devoted to modeling experimental conditions, and based on the obtained results, a detailed redox mechanism of the investigated analyte was proposed. This represents the first complete and unambiguous elucidation of the FNT redox mechanism, supported by joined experimental and theoretical data. Square wave voltammetry (SWV) was utilized for quantification, whereby the FNT oxidation peak was chosen for monitoring the analyte concentration. The developed sensor provided a nanomolar detection limit (3.2 nmol L⁻¹), a wide linear concentration range (from 0.01 to 13.7 μmol L⁻¹), and good precision, repeatability, and selectivity towards FNT. Practical application possibility was explored by testing the sensor performance for examining tap water and apple samples. Recovery tests, conducted during the FNT-spiked sample assays, showed a great application capability of the developed sensor for real-time monitoring of FNT traces in environmental samples.

Authors: Slađana Đurđić, Filip Vlahović, Miloš Ognjanović, Pavol Gemeiner, Olha Sarahman, Vesna Stanković, Jelena Mutić, Dalibor Stanković, Ľubomír Švorc

Full Source: The Science of the total environment 2023 Nov 15:909:168483. doi: 10.1016/j.scitotenv.2023.168483.

Reporting and reproducibility: Proteomics of fish models in environmental toxicology and ecotoxicology

2023-11-16

Environmental toxicology and ecotoxicology research efforts are employing proteomics with fish models as New Approach Methodologies, along with in silico, in vitro and other omics techniques to elucidate hazards of toxicants and toxins. We performed a critical review of toxicology studies with fish models using proteomics and reported fundamental parameters across experimental design, sample preparation, mass spectrometry, and bioinformatics of fish, which represent alternative vertebrate models in environmental toxicology, and ecotoxicology. We observed inconsistencies in reporting and methodologies among experimental designs, sample preparations, data acquisitions and bioinformatics, which can affect reproducibility of experimental results. We identified a distinct need to develop reporting guidelines for proteomics use in environmental toxicology and ecotoxicology, increased QA/QC throughout studies, and method optimization with an emphasis on reducing inconsistencies among studies. Several recommendations are offered as logical steps to advance development and application of this

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emerging research area to understand chemical hazards to public health and the environment.

Authors: Abigail N Henke, Srihar Chilukuri, Laura M Langan, Bryan W Brooks

Full Source: The Science of the total environment 2023 Nov 16:168455. doi: 10.1016/j.scitotenv.2023.168455.

PHARMACEUTICAL/TOXICOLOGY

Adverse impacts of environmentally relevant PFOS alternatives on mice pancreatic tissues

2023-11-17

Perfluorooctane sulfonate (PFOS) alternatives are chemicals that are used to make a range of products. Researchers have found that PFOS alternatives are probably no less toxic than PFOS, which has aroused concern. It has also revealed that the pancreas may be harmed by exposure to PFOS alternatives. However, there is insufficient evidence to demonstrate the toxicity mechanisms of PFOS alternatives. This study demonstrates the adverse effects of three PFOS alternatives on the pancreatic health of mice. After subchronic exposure to PFOS alternatives at environmentally relevant concentrations (800 µg/L perfluorohexanesulfonate, 800 µg/L perfluorobutanesulfonate, and 3 µg/L sodium *p*-perfluorooctanoate) via drinking water for 6 weeks, toxicity mechanisms were elucidated by examining histopathology, immunity, endoplasmic reticulum stress, 16S rRNA, and short-chain fatty acid targeted metabolomics. Sodium *p*-perfluorooctanoate significantly increased levels of TNF- α , IL-6, *p*-PERK, and ATF-4 and decreased the abundance of Akkermansia muciniphila and Lactobacillus reuteri. In addition, the three PFOS alternatives changed the composition of the gut microbiota in mice. Short-chain fatty acids, which are metabolites of the gut microbiota, also significantly decreased. Correlation analysis demonstrates that the alteration of gut microbes is related to the adverse effects on the mice pancreas. Results suggest that the murine pancreas may be toxic endpoints of PFOS alternatives. This study alerts the threats to human health and accelerates the toxicology research of an increasing number of emerging PFOS alternatives.

Authors: Lihui Zhao, Miaomiao Teng, Di Shi, Jiaqi Sun, Yunxia Li, Zixuan Zhang, Wentao Zhu, Fengchang Wu

Full Source: The Science of the total environment 2023 Nov 17:909:168649. doi: 10.1016/j.scitotenv.2023.168649.

Perfluorooctane sulfonate (PFOS) alternatives are chemicals that are used to make a range of products.

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Long-term exposure to polystyrene microplastics induces hepatotoxicity by altering lipid signatures in C57BL/6J mice

2023-11-16

It is estimated that the life of plastics is hundreds to thousands of years, their lasting properties making plastic debris absorbing toxic chemicals and degrading into microplastics (MPs). The purpose of this study was to explore the effects of exposure to different size (0.08 and 0.5 µm) polystyrene (PS) in mice. After 16 weeks of exposure, it was found that PS-MPs could be identified in the liver. No effect of PS-MPs treatment on body weight was observed. PS-MPs exposure disturbed lipids and lipid-like molecule metabolisms and perturbed the citrate cycle and oxidative phosphorylation. Meanwhile, isocitrate dehydrogenase (ICDHc), nicotinamide adenine dinucleotide -malate dehydrogenase (NAD-MDH), succinate dehydrogenase (SDH), α ketoglutarate dehydrogenase (α -KGDH) activities and adenosine triphosphate (ATP) level were obviously affected by PS-MPs treatment. In addition, significant differences were recorded in catalase (CAT) and malondialdehyde (MDA) levels, indicating that PS-MPs exposure induced an oxidative stress in the liver. In conclusion, our present study provided the first evidence of: (a) long-term exposure to PS-MPs lead to PS-MPs accumulated in the liver and results in liver injury; (b) long-term exposure to PS-MPs disturbs lipids and lipid-like molecule metabolisms; (c) long-term exposure to PS-MPs perturbs citrate cycle and oxidative phosphorylation and leads to oxidative stress in the liver.

Authors: Jiawen Tao, Ping Deng, Min Lin, Chunhai Chen, Qinlong Ma, Lingling Yang, Wenjuan Zhang, Yan Luo, Siyu Chen, Huifeng Pi, Zhou Zhou, Zhengping Yu

Full Source: Chemosphere 2023 Nov 16:347:140716. doi: 10.1016/j.chemosphere.2023.140716.

It is estimated that the life of plastics is hundreds to thousands of years, their lasting properties making plastic debris absorbing toxic chemicals and degrading into microplastics (MPs).

Binary metal oxide (NiO/SnO₂) composite with electrochemical bifunction: Detection of neuro transmitting drug and catalysis for hydrogen evolution reaction

2023-11-17

The synergetic effect between dual oxides in binary metal oxides (BMO) makes them promising electrode materials for the detection of toxic chemicals, and biological compounds. In addition, the interaction between the cations and anions of diverse metals in BMO tends to create more oxygen vacancies which are beneficial for energy storage devices. However, specifically targeted synthesis of BMO is still arduous. In this work, we prepared a nickel oxide/tin oxide composite (NiO/SnO₂)

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through a simple solvothermal technique. The crystallinity, specific surface area, and morphology were fully characterized. The synthesized BMO is used as a bifunctional electrocatalyst for the electrochemical detection of dopamine (DPA) and for the hydrogen evolution reaction (HER). As expected, the active metals in NiO/SnO₂ composite afforded a higher redox current at a reduced redox potential with a nanomolar level detection limit (4 nm) and excellent selectivity. Moreover, a better recovery rate is achieved in the real-time detection of DPA in human urine and DPA injection solution. Compared to other metal oxides, NiO/SnO₂ composite afforded lower overpotential (157 mV @10 mA cm⁻²), Tafel slope (155 mV dec⁻¹), and long-term durability, with a minimum retention rate. These studies conclude that NiO/SnO₂ composite can act as a suitable electrode modifier for electrochemical sensing and the HER.

Authors: Balamurugan Muthukutty, Thang Cao Doan, Hyojong Yoo
Full Source: Environmental research 2023 Nov 17:117655. doi: 10.1016/j.envres.2023.117655.

OCCUPATIONAL

The impact of short-term exposures to ambient NO₂, O₃, and their combined oxidative potential on daily mortality

2023-11-17

It is widely recognized that air pollution exerts substantial detrimental effects in human health and the economy. The potential for harm is closely linked to the concentrations of pollutants like nitrogen dioxide (NO₂) and ozone (O₃), as well as their collective oxidative potential (OX). Yet, due to the challenges of directly monitoring OX as an independent factor and the influences of different substances' varying ability to contain or convey OX, uncertainties persist regarding its actual impact. To provide further evidence to the association between short-term exposures to NO₂, O₃, and OX and mortality, this study conducted multi-county time-series analyses with over-dispersed generalized additive models and random-effects meta-analyses to estimate the mortality data from 2014 to 2020 in Jiangsu, China. The findings reveal that short-term exposures to these pollutants are linked to increased risks of all-cause, cardiovascular, and respiratory mortality, where NO₂ demonstrates 2.11% (95% confidence interval: 1.79%, 2.42%), 2.28% (1.91%, 2.66%), and 2.91% (2.13%, 3.69%) respectively per every 10 ppb increase in concentration, and the effect of O₃ is 1.11% (0.98%, 1.24%), 1.39% (1.19%, 1.59%), and 1.82% (1.39%, 2.26%), and OX is 1.77% (1.58%, 1.97%), 2.19% (1.90%, 2.48%), and 2.90% (2.29%, 3.52%). Notably, women and individuals aged over 75 years exhibit

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higher susceptibility to these pollutants, with NO₂ showing a greater impact, especially during the warm seasons. The elevated mortality rates associated with NO₂, O₃, and OX underscore the significance of addressing air pollution as a pressing public health issue, especially in controlling NO₂ and O₃ together. Further research is needed to explore the underlying mechanisms and possible influential factors of these effects.

Authors: Ziqi Tang, Jianhui Guo, Jinyi Zhou, Hao Yu, Yaqi Wang, Xinyao Lian, Jin Ye, Xueqiong He, Renqiang Han, Jing Li, Shaodan Huang
Full Source: Environmental research 2023 Nov 17:241:117634. doi: 10.1016/j.envres.2023.117634.

Population pharmacokinetic/pharmacodynamic modeling and exposure-response analysis of ciprofol in the induction and maintenance of general anesthesia in patients undergoing elective surgery: A prospective dose optimization study

2023-11-15

Aim: This study aimed to establish a population pharmacokinetic and pharmacodynamic (PK-PD) model to explore the optimal maintenance dose and appropriate starting time of maintenance dose after induction of ciprofol and investigate the efficacy and safety of ciprofol for general anesthesia induction and maintenance in patients undergoing elective surgery.

Method: A total of 334 subjects with 3092 concentration measurements from nine clinical trials and 115 subjects with 5640 bispectral index (BIS) measurements from two clinical trials were used in the population PK-PD analysis. Exposure-response relationships for both efficacy endpoints (duration of anesthesia successful induction, time to recovery from anesthesia, time to respiratory recovery, and time from discontinuation to the 1st/3rd consecutive Aldrete score \geq 9) and safety variables (hypotension, bradycardia, and injection site pain) were evaluated based on the data gathered from 115 subjects in two clinical trials.

Result: Ciprofol pharmacokinetics (PK) were adequately described by a three-compartment model with first-order elimination from the central compartment and redistribution from the deep and shallow peripheral compartments. An inhibitory sigmoidal E_{max} model best described the relationship between ciprofol effect-site concentrations and BIS measurements. Body weight, age, sex, blood sampling site, and study type (short-term infusion vs long-term infusion) were identified as statistically

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significant covariates on the PK of ciprofol. No covariates were found to have a significant effect on the pharmacodynamic (PD) parameters. The PK-PD simulation results showed that the optimal maintenance dose was 0.8 mg/kg/h and the appropriate time to start the maintenance dose was 4-5 mins after the induction dose of ciprofol. Within the exposure range of this study, no meaningful correlations between ciprofol exposures and efficacy or safety endpoints were observed.

Conclusion: A population PK-PD model was successfully developed to describe the ciprofol PK and BIS changes. Efficacy was consistent across the exposure range with a well-tolerated safety profile indicating no maintenance dose adjustment is required for patients undergoing elective surgery.

Authors: Lu Liu, Kun Wang, Yuting Yang, Mengyue Hu, Meixia Chen, Xiao Liu, Pangke Yan, Nan Wu, Xiaoqiang Xiang

Full Source: Journal of clinical anesthesia 2023 Nov 15:92:111317. doi: 10.1016/j.jclinane.2023.111317.