

April 15, 2005

# ENVIRONMENTAL Science & Technology

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## Isotopic Constraints on the Fate of PETROLEUM RESIDUES Sequestered in Salt Marsh Sediments

Accounting for Differences in Estrogenic  
Responses in Rainbow Trout and Roach

An Introduction to the National  
Environmental Methods Index

PUBLISHED BY  
THE AMERICAN  
CHEMICAL SOCIETY

## Research

### Characterization of Natural and Affected Environments

#### ■ 2417

#### Characterization of Trophic Transfer for Polychlorinated Dibenzo-*p*-dioxins, Dibenzofurans, Non- and Mono-ortho Polychlorinated Biphenyls in the Marine Food Web of Bohai Bay, North China

Yi Wan, Jianying Hu, Min Yang, Lihui An, Wei An, Xiaohui Jin, Tatsuya Hattori, and Mitsuaki Itoh

The trophic transfer is determined of 9 dibenzo-*p*-dioxin, 11 dibenzofuran, and 12 non- and mono-ortho-polychlorinated biphenyl congeners in a marine food web.

#### ■ 2426

#### Wet Deposition of Persistent Organic Pollutants to the Global Oceans

Elena Jurado, Foday Jaward, Rainer Lohmann, Kevin C. Jones, Rafael Simó, and Jordi Dachs

Spatial distribution and seasonal trends of wet deposition fluxes of POPs to the oceans are predicted by combining field measurements of atmospheric POPs and remote sensing.

#### ■ 2436

#### Time Trends of Atmospheric PBDEs Inferred from Archived U.K. Herbage

Ashraf Hassanin, A. E. Johnston, Gareth O. Thomas, and Kevin C. Jones

Analysis of samples from Rothamsted Experimental Station between 1930 and 2004 shows a rise through the 1970s and a recent decline.

#### 2442

#### Corrosion of Unexploded Ordnance in Soil—Field Results

Michael D. Chendorain, Lloyd D. Stewart, and Bonnie Packer

This paper provides results of UXO corrosion from a field survey of 14 inactive army ranges distributed throughout the mainland United States.

#### 2448

#### Synergic Effect of Gold Mining and Damming on Mercury Contamination in Fish

Alain Boudou, Régine Maury-Brachet, Marina Coquery, Gilles Durrieu, and Daniel Cossa

Mercury from gold mining alone is not sufficient to account for high concentrations in fish; conditions that favor methylation, such as anoxia within hydroelectric reservoirs, are needed.

#### 2455

#### Analysis of Oxidative DNA Damage 8-Hydroxy-2'-deoxyguanosine as a Biomarker of Exposures to Persistent Pollutants for Marine Mammals

Chi-Shan Li, Kuen-Yuh Wu, Gou-Ping Chang-Chien, and Chin-Cheng Chou

8-OHdG is studied as an oxidative damage biomarker for marine mammals.

#### 2461

#### Mixtures of Estrogenic Contaminants in Bile of Fish Exposed to Wastewater Treatment Works Effluents

R. Gibson, M. D. Smith, C. J. Spary, C. R. Tyler, and E. M. Hill

Fish exposed to effluents from wastewater treatment works bioconcentrate a complex mixture of estrogenic contaminants, including a "new" environmental estrogen, 17 $\beta$ -dihydroequilenin.

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#### 2472

#### Novel Flame-Retardants, 1,2-Bis(2,4,6-tribromophenoxy)-ethane and 2,3,4,5,6-Pentabromoethylbenzene, in United States' Environmental Samples

Eunha Hoh, Lingyan Zhu, and Ronald A. Hites

Two brominated flame retardants are identified in outdoor air and sediment samples from the Great Lakes region with GC/MS and authentic reference materials.

#### 2478

#### Characterization of Colloidal and Humic-Bound Ni and U in the "Dissolved" Fraction of Contaminated Sediment Extracts

Brian P. Jackson, James F. Ranville, Paul M. Bertsch, and Andrew G. Sowder

Uranium in contaminated sediment-water extracts is bound to a colloidal phase and dissolved organic matter, whereas nickel is present as the free cation or as labile complexes.

#### ■ 2486

#### Boron Isotopes in the Seine River, France: A Probe of Anthropogenic Contamination

Benjamin Chetelat and Jérôme Gaillardet

Boron isotopic ratios are used to identify contamination sources in surface waters of a watershed strongly impacted by human activities.

#### 2494

#### Organochlorine Pesticides in Agricultural Soil and Vegetables from Tianjin, China

S. Tao, F. L. Xu, X. J. Wang, W. X. Liu, Z. M. Gong, J. Y. Fang, L. Z. Zhu, and Y. M. Luo

Differences in HCHs and DDXs between rhizosphere and bulk soils depend on soil organic matter; roots of fibrous vegetables absorbed more pesticides than tuberous vegetables did.

### Environmental Processes

#### 2500

#### Detachment-Influenced Transport of an Adhesion-Deficient Bacterial Strain within Water-Reactive Porous Media

Meiping Tong, Xiqing Li, Christina N. Brow, and William P. Johnson

Shapes of profiles of retained microspheres and bacteria in porous media differ depending on system conditions and demonstrate the influence of detachment under some conditions.

#### 2509

#### Copper–Glyphosate Sorption to Microcrystalline Gibbsite in the Presence of Soluble Keggin Al<sub>13</sub> Polymers

William E. Dubbin and Garrison Sposito

Incorporation of Al<sub>13</sub> tridecamers into model copper-glyphosate–gibbsite systems induces abrupt solubilization of copper and glyphosate near pH 6, coincident with Al<sub>13</sub> deprotonation.

■ Supporting information is available free at <http://pubs.acs.org/est>.

**■ 2515****Low Molecular Weight Carboxylic Acids in Oxidizing Porphyry Copper Tailings**

Bernhard Dold, David W. Blowes, Ralph Dickhout, Jorge E. Spangenberg, and Hans-Rudolf Pfeifer

Metabolic byproducts of bacterial activity in porphyry copper mine tailings trigger Fe(III) reduction and increase iron mobility through low-molecular-weight carboxylic acids and Fe(III)-Fe(II) cycling.

**■ 2522****Quantifying the Contribution of Different Sorption Mechanisms for 2,4-Dichlorophenoxyacetic Acid Sorption by Several Variable-Charge Soils**

Seunghun Hyun and Linda S. Lee

Hydrophilic 2,4-D sorption by variable-charge soils is mainly determined by anion exchange and calcium bridging.

**■ 2529****Role for Fe(III) Minerals in Nitrate-Dependent Microbial U(IV) Oxidation**

John M. Senko, Yasser Mohamed, Thomas A. Dewers, and Lee R. Krumholz

Nitrate-dependent U(IV) oxidation is mediated by iron and dependent on Fe(III) mineralogy.

**■ 2537****Arsenate Adsorption Mechanisms at the Allophane-Water Interface**

Yuji Arai, D. L. Sparks, and J. A. Davis

Arsenate readily adsorbs on allophane via ligand exchange mechanisms, and the inner-sphere bidentate, binuclear surface species on aluminum octahedral structures persist with increasing residence time.

**■ 2545****Isotopic Constraints on the Fate of Petroleum Residues Sequestered in Salt Marsh Sediments**

Helen K. White, Christopher M. Reddy, and Timothy I. Eglinton

Naturally abundant radiocarbon is an inverse tracer of fossil-fuel-derived carbon in marine sediments.

**■ 2552****Determination of Microbial Carbon Sources in Petroleum Contaminated Sediments Using Molecular  $^{14}\text{C}$  Analysis**

Gregory F. Slater, Helen K. White, Timothy I. Eglinton, and Christopher M. Reddy

$^{14}\text{C}$  analysis of individual phospholipid fatty acids reveals that microbial metabolism of petroleum residues in contaminated marsh sediments is insignificant.

**■ 2559****Vehicle Self-Pollution Intake Fraction: Children's Exposure to School Bus Emissions**

Julian D. Marshall and Eduardo Behrentz

Inhalation intake of emissions is much lower if reductions come from a school bus compared with other types of vehicles.

**■ 2564****Decrease in Net Mercury Methylation Rates Following Iron Amendment to Anoxic Wetland Sediment Slurries**

Anna S. Mehrotra and David L. Sedlak

Decreases in net mercury methylation in estuarine wetland sediment slurries following iron(II) addition suggest that iron addition might be a viable strategy for minimizing mercury methylation in engineered wetland sediments.

**■ 2571****Polycyclic Aromatic Hydrocarbon Biodegradation Rates: A Structure-Based Study**

Kristine H. Wammer and Catherine A. Peters

Biodegradation rates for 22 2–4-ring PAHs are measured, and their molecular structure is examined.

**■ 2579****Oxidation of Fe(II) in Rainwater**

J. D. Willey, R. F. Whitehead, R. J. Kieber, and D. R. Hardison

Photochemically produced Fe(II) in rain can be oxidized by hydrogen peroxide within hours; however, other forms of Fe(II) in rain are much more stable.

**■ 2586.****Mechanism of Interactions between Hg(II) and Demeton S: An NMR Study**

Simo O. Pehkonen and Zaher M. A. Judeh

$^1\text{H}$  and  $^{31}\text{P}$  NMR spectroscopy is used in the first *in situ* study of the molecular interactions between an aqueous solution of Hg(II) and Demeton S, an organophosphorus pesticide.

**■ 2592****Effects of pH and Cationic and Nonionic Surfactants on the Adsorption of Pharmaceuticals to a Natural Aquifer Material**

Ajai C. Hari, Rajiv A. Paruchuri, David A. Sabatini, and Tohren C. G. Kibbey

Batch adsorption experiments are used to examine the effects of pH and surfactants on the adsorption behavior of four pharmaceutical compounds.

**■ 2599****Accounting for Differences in Estrogenic Responses in Rainbow Trout (*Oncorhynchus mykiss*: Salmonidae) and Roach (*Rutilus rutilus*: Cyprinidae) Exposed to Effluents from Wastewater Treatment Works**

C. R. Tyler, C. Spary, R. Gibson, E. M. Santos, J. Shears, and E. M. Hill

Fish species show differences in their responsiveness to estrogenic effluents from wastewater treatment works.

**■ 2608****Interfacial Interactions between Np(V) and Manganese Oxide Minerals Manganite and Hausmannite**

P. A. Wilk, D. A. Shaughnessy, R. E. Wilson, and H. Nitsche

Manganese minerals manganite and hausmannite sorb pentavalent plutonium, but problems arise in characterizing the sorbed species by XAS because of high beam intensities.

**■ 2616****Enzymatic versus Nonenzymatic Conversions during the Reduction of EDTA-Chelated Fe(III) in BioDeNO<sub>x</sub> Reactors**

Peter van der Maas, Shen Peng, Bram Klapwijk, and Piet Lens

Biological reduction of EDTA-chelated Fe(III), a core reaction in BioDeNO<sub>x</sub> reactors, is mediated by an electron-shuttling compound, presumably polysulfide.

**■ 2624****Cell-Membrane Damage and Element Leaching in Transplanted *Parmelia sulcata* Lichen Related to Ambient SO<sub>2</sub>, Temperature, and Precipitation**

Ana P. Marques, Maria C. Freitas, Hubert T. Wolterbeek, Olav M. Steinebach, Tona Verburg, and Jeroen J. M. De Goeij

Lichen vitality in large geographical areas may be governed by the area's variability in temperature and precipitation rather than by variability in metal deposition rates.

**2631**

**Reductive Dechlorination of Tetrachloroethene to *trans*-Dichloroethene and *cis*-Dichloroethene by PCB-Dechlorinating Bacterium DF-1**

Gregory S. Miller, Charles E. Milliken, Kevin R. Sowers, and Harold D. May  
PCB-dechlorinating bacterium DF-1 dechlorinates PCE and TCE to *trans*- and *cis*-DCE.

**2636**

**Settling Behavior of Unpurified *Cryptosporidium* Oocysts in Laboratory Settling Columns**

Pamela L. Young and Simeon J. Komisar

Settling velocity of unpurified *Cryptosporidium* oocysts in columns ranges from 0.22 to 1.78  $\mu\text{m}/\text{s}$ .

**2645**

**Reduction of Organically Complexed Ferric Iron by Superoxide in a Simulated Natural Water**

Andrew L. Rose and T. David Waite

Superoxide is an effective reductant of ferric iron complexed to natural organic matter in seawater; this process could increase iron bioavailability.

**2651**

**Cryogenic Laser Induced U(VI) Fluorescence Studies of a U(VI) Substituted Natural Calcite: Implications to U(VI) Speciation in Contaminated Hanford Sediments**

Zheming Wang, John M. Zachara, James P. McKinley, and Steven C. Smith  
Time-resolved laser-induced fluorescence spectroscopy and imaging spectromicroscopy studies indicate the presence of U(VI)-incorporated aragonite and calcite in both natural calcite and uranium-contaminated Hanford sediments.

**2660**

**Interaction of Tetracycline with Aluminum and Iron Hydrous Oxides**

Cheng Gu and K. G. Karthikeyan

The role of aluminum and iron hydrous oxides in influencing the environmental reactivity of tetracycline, a widely used antibiotic compound, is reported.

**2668**

**Secondary Organic Aerosol Formation by Irradiation of 1,3,5-Trimethylbenzene- $\text{NO}_x-\text{H}_2\text{O}$  in a New Reaction Chamber for Atmospheric Chemistry and Physics**

Dwane Paulsen, Josef Dommen, Markus Kalberer, André S. H. Prévôt, René Richter, Mirjam Sax, Martin Steinbacher, Ernest Weingartner, and Urs Baltensperger

A fluorinated, ethylene-propylene bag suspended in a temperature-controlled enclosure with four xenon arc lamps is used to irradiate primary gas components.

**2679**

**Characterization of Adsorption Sites on Aggregate Soil Samples Using Synchrotron X-ray Computerized Microtomography**

Susan J. Altman, Mark L. Rivers, Marissa D. Reno, Randall T. Cygan, and Angela A. McLain

CMT is used to determine the relative amounts of iron oxyhydroxides and iron-bearing clays and to delineate the relationship of cesium adsorption with iron-bearing materials within soil aggregate samples.

**2686**

**Some Sources and Sinks of Monomethyl and Inorganic Mercury on Ellesmere Island in the Canadian High Arctic**

Vincent L. St. Louis, Martin J. Sharp, Alexandra Steffen, Al May, Joel Barké, Jane L. Kirk, David J. A. Kelly, Shelley E. Arnott, Bronwyn Keatley, and John P. Smol

Atmospheric mercury depletion events result in little net mercury deposition to Arctic snowpacks, whereas northern oceans may be an ultimate source of methylmercury to snowpacks.

## Environmental Modeling

**2702**

**Estimating Partition Coefficients for Fuel-Water Systems: Developing Linear Solvation Energy Relationships Using Linear Solvent Strength Theory To Handle Mixtures**

J. Samuel Arey and Philip M. Gschwend

LSST is used to combine existing solvent-water LSERs; this allows good estimates of fuel-water mixtures partitioning to be made for both polar and nonpolar solutes.

**2711**

**Five-Stage Environmental Exposure Assessment Strategy for Mixtures: Gasoline as a Case Study**

Karen L. Foster, Don Mackay, Thomas F. Parkerton, Eva Webster, and Lynne Milford

An exposure assessment strategy for mixtures is presented and illustrated by application to gasoline hydrocarbons.

**2719**

**Halogen Substitution Patterns among Disinfection Byproducts in the Information Collection Rule Database**

Alexa Obolensky and Philip C. Singer

Multivariate analysis and a new DBP halogen substitution metric are used to demonstrate strong interclass correlations in bromine substitution, and these are applied to quality assurance.

**2731**

**Determination of the Fractal Dimension of Microbial Flocs from the Change in Their Size Distribution after Breakage**

Xiao-yan Li and Ruby P. C. Leung

The fractal dimension of activated sludge flocs can be determined from the change in their particle size distribution brought about by enhanced breakage.

**2736**

**Degradation of Biological Weapons Agents in the Environment: Implications for Terrorism Response**

Amy L. Stuart and Dean A. Wilkening

Degradation of biological weapons agents in the environment is reviewed and modeled to determine impacts on terrorism response and response planning.

## Environmental Measurements Methods

**2744**

**Partition of Endocrine-Disrupting Chemicals between Colloids and Dissolved Phase as Determined by Cross-Flow Ultrafiltration**

Ruixia Liu, Andrew Wilding, Andrew Hibberd, and John L. Zhou

Dynamic sorption of endocrine-disrupting chemicals by river colloids is determined by cross-flow ultrafiltration coupled with GC/MS.

**2753**

**New Analytical Method for the Determination of Levoglucosan, Polyhydroxy Compounds, and 2-Methylerythritol and Its Application to Smoke and Rainwater Samples**

G. Schkolnik, A. H. Falkovich, Y. Rudich, W. Maenhaut, and P. Artaxo

With water extraction and ion-exclusion HPLC detection at 194 nm, the method broadens the speciation possibilities offered by simple HPLC.

■ Supporting information is available free at <http://pubs.acs.org/est>.

**2762**

► **In Vivo Visual Reporter System for Detection of Estrogen-Like Substances by Transgenic Medaka**

Kanta Kurauchi, Yoshitsugu Nakaguchi, Makiko Tsutsumi, Hiroshi Hori, Ryo Kurihara, Shinya Hashimoto, Ryoko Ohnuma, Yoshihiko Yamamoto, Sumiko Matsuoka, Shin'ichiro Kawai, Takashi Hirata, and Masato Kinoshita

Visual detection of estrogen-like substances with transgenic medaka is studied.

**2769**

**Microbenthic Chamber with Microelectrode for In-Situ Determination of Fluxes of Dissolved S(–II), I<sup>–</sup>, O<sub>2</sub>, Mn, and Fe**

Conrad S. Chapman and Constant M. G. van den Berg

A 2-mL benthic chamber fitted with a microelectrode for voltammetric detection is used to determine benthic fluxes of oxygen, sulfide, iodide, and manganese within minutes.

■ **2777**

**Quantitative RT-PCR Methods for Evaluating Toxicant-Induced Effects on Steroidogenesis Using the H295R Cell Line**

Xiaowei Zhang, Richard M. K. Yu, Paul D. Jones, Gabriel K. W. Lam, John L. Newsted, Tannia Gracia, Markus Hecker, Klara Hilscherova, J. Thomas Sanderson, Rudolf S. S. Wu, and John P. Giesy

The results of this study indicate that the H295R cell line is appropriate for a transcriptometric screening assay for the effects of chemicals on steroidogenesis.

**2786**

**Evaluation of a Novel Malathion Immunoassay for Groundwater and Surface Water Analysis**

Eva M. Brun, Marta Garcés-García, Ma. José Bañuls, José A. Gabaldón, Rosa Puchades, and Ángel Maquieira

The development and application are presented of a specific immunoanalytical method to determine malathion residues in groundwaters and surface waters.

■ **2795**

**Solid-Phase Microextraction Measurement of Parent and Alkyl Polycyclic Aromatic Hydrocarbons in Milliliter Sediment Pore Water Samples and Determination of KDOC Values**

Steven B. Hawthorne, Carol B. Grabanski, David J. Miller, and Joseph P. Kreitinger

SPME provides a robust and sensitive method for determining parent and alkyl PAHs in sediment pore water at sensitivities needed to estimate hydrocarbon narcosis.

## Remediation and Control Technologies

**2804**

**Solid Waste Removes Toxic Liquid Waste: Adsorption of Chromium(VI) by Iron Complexed Protein Waste**

Nishtar Nishad Fathima, Rathinam Aravindhan, Jonnalagadda Raghava Rao, and Balachandran Unni Nair

This study explores the use of iron-complexed protein wastes from a tannery for the removal of chromium(VI).

**2811**

**Formation of Soluble Organo-Chromium(III) Complexes after Chromate Reduction in the Presence of Cellular Organics**

Geoffrey J. Puzon, Arthur G. Roberts, David M. Kramer, and Luying Xun  
Soluble organo-Cr(III) complexes are formed from Cr(VI) reduction in the presence of cellular organic metabolites.

**2818**

**Formation and Characterization of Aerobic Granules in a Sequencing Batch Reactor Treating Soybean-Processing Wastewater**

Kui-Zu Su and Han-Qing Yu

Formation of granules is a four-phase process, fitting well to a modified Logistic model that can estimate maximum diameter, lag time, and diameter growth rate.

■ **2828**

**Optimization of Coagulation–Flocculation Process for Palm Oil Mill Effluent Using Response Surface Methodology**

A. L. Ahmad, S. Ismail, and S. Bhatia

Response surface methodology is used for optimization of the coagulation–flocculation process for palm oil mill effluent.

■ **2835**

**Bench-Scale Investigation of Permanganate Natural Oxidant Demand Kinetics**

Kevin G. Mumford, Neil R. Thomson, and Richelle M. Allen-King

At least two reaction rates characterize the kinetics of permanganate reaction with naturally present reduced species in low-carbon-content aquifer solids.

**2841**

**Selective Catalytic Reduction of Nitrogen Oxides from Exhaust of Lean Burn Engine over In-Situ Synthesized Cu-ZSM-5/Cordierite**

Li Landong, Chen Jixin, Zhang Shujuan, Zhang Fuxiang, Guan Naijia, Wang Tianyou, and Liu Shuliang

Monolithic catalysts Cu-ZSM-5/cordierite and LaCu-ZSM-5/cordierite exhibit good reduction of exhaust NO<sub>x</sub> from an actual lean-burn gasoline engine; factors influencing catalytic activity are discussed.

**2848**

**Laboratory Studies of Electrochemical Treatment of Industrial Azo Dye Effluent**

Sanjay S. Vaghela, Ashok D. Jethva, Bhavesh B. Mehta, Sunil P. Dave, Subbarayappa Adimurthy, and Gadde Ramachandraiah

Decolorization and COD reduction in an azo dye wastewater are investigated under single-pass conditions at a dimensionally stable anode in a thin electrochemical flow reactor.

■ **2856**

**Sorption of <sup>243</sup>Am(III) to Multiwall Carbon Nanotubes**

Xiangke Wang, Changlun Chen, Wenping Hu, Aiping Ding, Di Xu, and Xiang Zhou

Multiwall carbon nanotubes adsorb <sup>243</sup>Am(III) with high efficiency via formation of stable complexes; sorption is strongly dependent on pH and weakly dependent on ionic strength.

**2861**

**Fluidized Bed Combustion Systems Integrating CO<sub>2</sub> Capture with CaO**

J. Carlos Abanades, Edward J. Anthony, Jinsheng Wang, and John E. Oakey  
Despite their limited performance as regenerable sorbents, natural limitations are suitable high-temperature sorbents for these systems because of their low price and availability.

■ **2867**

**Longevity of Granular Iron in Groundwater Treatment Processes: Corrosion Product Development**

Tamar Kohn, Kenneth J. T. Livi, A. Lynn Roberts, and Peter J. Vikesland  
X-ray diffraction, electron microscopy, electron energy loss spectroscopy, and micro-Raman spectroscopy are used to examine corrosion product development on granular iron surfaces exposed to different water constituents.

■ **2880**

**Addition of Activated Carbon to Sediments to Reduce PCB Bioaccumulation by a Polychaete (*Neanthes arenaceodentata*) and an Amphipod (*Leptocheirus plumulosus*)**

Rod N. Millward, Todd S. Bridges, Upal Ghosh, John R. Zimmerman, and Richard G. Luthy

Mixing activated carbon into contaminated sediment is a new, *in situ* treatment method that reduces the biouptake of PCBs by benthic organisms.

**2888**

### **Laboratory Study of Treatment of Trichloroethene by Chemical Oxidation Followed by Bioremediation**

Leila Hrapovic, Brent E. Sleep, David J. Major, and Eric D. Hood

Column studies with soils and emplaced TCE sources demonstrate the feasibility of remediation of TCE source zones with permanganate flushing followed by biostimulation and bio-augmentation.

**2898**

### **Assessment of the Energy Dissipation Parameters Inside the Draft Tube of a Liquid Spout-Fluid Bed**

Ayşe Çeçen Erbil and Mustafa Turan

A theoretical model assesses the possibility of applying draft tubes in filter backwashing by calculating the energy dissipation parameters inside a draft tube.

**2906**

### **Electrodialytic Removal of Cu, Zn, Pb, and Cd from Harbor Sediment: Influence of Changing Experimental Conditions**

Gunvor M. Nystroem, Lisbeth M. Ottosen, and Arne Villumsen

An electric field is applied to stirred sediment suspensions to remove heavy metals from contaminated harbor sediments.

## **Additions and Corrections**

**2912**

### **Storm Disturbance of Sediment Contaminants at a Hot-Spot in the Baltic Sea Assessed by $^{234}\text{Th}$ Radionuclide Tracer Profiles**

Michael Kersten, Thomas Leipe, and Franz Tauber

- Supporting information is available free at <http://pubs.acs.org/est>.
- ▶ This issue contains a news story about this research.