

**9:00 182.** Development and characterization of cyclic analogs of apelin-13 through replica-exchange molecular dynamics and experimental validation.

**N. J. M. Macaluso**, S. L. Pitkin, P. N. Sanderson, A. P. Davenport, R. C. Glen

**9:30 183.** E-*Novo* automated workflow for structure-based lead optimization.

**B. C. Pearce**, D. R. Langley, J. Kang, H. Huang, A. Kulkarni

**10:00 184.** Hepatitis B virus DNA polymerase inhibition: Computational insight into resistance development. **P. R. Daga**, R. J. Doerksen

**10:30** Intermission.

**10:40 185.** Good BREEDing, techniques for generating hybrid molecules.

**J. M. Leonard**

**11:10 186.** Ro5.1: Pfizer rules revisited.

**T. I. Oprea**

**11:40 187.** Graph representation of molecular datasets: Applications to dataset visualization and comparison using graph indices. **D. Fourches**, A. Tropsha

**Adaptive Scoring Functions** Sponsored by CINP, Cosponsored by the CSA Trust and COMP

### WEDNESDAY AFTERNOON

Section B

Salt Palace Convention Center  
257

#### Drug Discovery

I. Visiers, *Organizer*

A. Tropsha, *Presiding*

**1:30 188.** Accurate prediction of logD and HERG liability by pharmacophore fingerprint QSAR (PFQQSAR) for drug discovery in GSK. **Z. Yang**, T.-Y. Wu

**189.** Withdrawn.

**2:00 190.** A novel method for generating structure-based pharmacophores using energetic analysis. **N. K. Salam**, B. W. Sherman

**2:30 191.** Alignment and overlay of protein surfaces using shape and chemical features: Application to detect local similarity among ligand binding sites. **B. K. Rai**, G. A. Bakken

**3:00** Intermission.

**3:10 192.** Automated QSAR modeling to guide drug design. **O. Obrezanova**, M. D. Segall

**3:40 193.** Combination of amide hydrogen/deuterium-exchange mass spectrometry and computational chemistry: Applications to study protein dynamics, protein-ligand interactions, and protein-protein interactions. **Y. Hamuro**, **D. Pandit**

**4:10 194.** Detecting conserved patterns of shape and property distributions on ligand binding site surfaces of proteins using property-encoded shape distributions. **S. Das**, A. Kokardekar, C. M. Breneman

Section C

Salt Palace Convention Center  
258

#### Quantum Chemistry Making the Difficult Attainable

A. E. Roitberg, *Organizer*

K. Shahrokh, *Presiding*

**1:30 195.** Accurate calculation of explicit water molecule free energies: Applications to PDZ binding domains. **T. Beuming**, B. W. Sherman, R. Farid

**2:00 196.** Statistics and physical origins of ionization state changes upon protein-ligand binding. **A. Onufriev**

**2:30 197.** A solution structural model for human intrinsic blood coagulation tenase complex (FVIIIa:flXa) derived from protein docking and MD simulations: Implications for factor X activation. **D. Venkateswari**

**3:00** Intermission.

**3:10 198.** Definition of chemical reactivity parameter and its validation. **S. Yao**

**3:40 199.** Cross Pharma High Performance Computing Forum: Collaboration to optimize HPC capabilities to accelerate drug discovery. **Z. Yang**

**4:10 200.** Lemniscular phyrins as calibrants of electron correlation fidelity in hybrid DFT methods. **H. S. Rzepa**

**Adaptive Scoring Functions** Sponsored by CINP, Cosponsored by the CSA Trust and COMP

### THURSDAY MORNING

Section A

Salt Palace Convention Center  
257

#### Quantum Chemistry The Quantum and Physical Worlds Meet

A. E. Roitberg, *Organizer*

R. J. Doerksen, *Presiding*

**8:30 201.** Acidity modeling of arsenic and arsenous oxide and sulfide acids using ab initio model chemistries.

**M. D. Zimmermann**, J. A. Tossell

**9:00 202.** Red shift vs. blue shift of C-H stretching frequency of C-H...π interactions in benzene dimer: Influence of counterpoise correction in the frequency calculations at the MP2 method.

**T. C. Dinadayalane**, J. Leszczynski

**9:30 203.** Density functional calculations of 15N chemical shielding in peptides and proteins. **L. Cai**, D. Fushman, D. Kosov

**10:00 204.** Nonlinear dimensionality reduction for reaction path discovery in ab initio multiple spawning dynamics.

**A. M. Virshup**, J. Chen, T. J. Martinez

**10:30** Intermission.

**10:40 205.** Spin decoherence in carbon and boron-nitride nanoribbons. **A. F. Izmaylov**, M. J. Frisch

**11:10 206.** Theoretical study of the anharmonicity of molecular vibrations of Li<sup>+</sup>-H<sub>2</sub>, Na<sup>+</sup>-H<sub>2</sub>, B<sup>+</sup>-H<sub>2</sub> and Al<sup>+</sup>-H<sub>2</sub> complexes.

**N. De Silva**, B. Njegic, M. S. Gordon

**11:40 207.** Calculation of quantum mechanical vibrational energy relaxation rates in liquids via semiclassical methods.

**F. X. Vázquez**, E. Geva

Section B

Salt Palace Convention Center  
258

#### Drug Discovery

I. Visiers, *Organizer*

Z. P. Yang, *Presiding*

**8:30 208.** eHITS: Docking and scoring ligand/target interactions to give good score-rmsd and ic50 correlations in *in silico* high throughput screening. **D. Harris**, Z. Szoldos

**9:00 209.** Mining public databases for structure-activity relationships. **B. Wendt**, U. Uhrig, L. Wang

**9:30 210.** Protein ensemble generation for improved ligand-protein docking.

**A. Nayeem**, K. A. Rossi, S. R. Kimura, S. R. Krystek Jr.

**10:00** Intermission.

**10:10 211.** Screening tools and results for inhibitors of human tyrosyl DNA phosphodiesterase (Tdp1). **I. E. Weidlich**, T. Dexheimer, Y. Pommier, C. Marchand, M. C. Nicklaus

**10:40 212.** Structure-based discovery and biological evaluation of novel selective TRAF6 inhibitors. **S. Zhang**, L. Du-Cuny, B. Darnay

**11:10 213.** Understanding the potential role of hydrogen bonding in drug discovery.

**D. C. Reuter**, K. Brameld, S. Connolly

### THURSDAY AFTERNOON

Section A

Salt Palace Convention Center  
257

#### Drug Discovery

I. Visiers, *Organizer*

B. J. Burke, *Presiding*

**1:00 214.** Computational approaches to antibacterial and antimalarial hit finding.

**A. P. Johnson**, C. W. G. Fishwick, G. A. McConkey, T. Heikkila, M. Davies, D. Cowan, A. Agarwal

**1:30 215.** Computer-aided design of [(biphenyloxy)propyl]isoxazoles – agents against coxsackievirus B3. **E. Muratov**, V. E. Kuz'min, A. G. Artemenko, E. Varlamova, A. Kuz'mina, A. Tropsha, V. Makarov, O. Riabova, P. Wutzler, M. Schmidtke

**2:00 216.** Docking and 3-D-QSAR studies on isatin sulfonamide analogs as caspase-3 inhibitors. **Q. Wang**, R. H. Mach, D. E. Reichert

**2:30** Intermission.

**2:40 217.** Prediction of cytochrome P450 mediated oxidation using induced fit docking. **M. Shelley**

**3:10 218.** Protein modeling and virtual screening to discover novel GSK-3 inhibitors. **P. Sivaprakasam**, P. R. Daga, A. Xie, **R. J. Doerksen**

**3:40 219.** Targeting the acetylcholine binding protein: A relaxed-complex approach to virtual screening. **A. Babakhani**, T. T. Talley, P. W. Taylor, J. A. McCammon

Section B

Salt Palace Convention Center  
258

#### Quantum Chemistry Materials. It's Where it's At!

A. E. Roitberg, *Organizer*

Y. Meng, *Presiding*

**1:00 220.** First-principles studies of octacyclopropylcubane: A novel high-energy density material. **S. L. Richardson**, R. N. Allen, D. Finkenstadt, M. J. Mehl, M. R. Pederson

**1:30 221.** Mechanism of thermal decomposition of carbamoyl phosphate and its stabilization by aspartate and ornithine transcarbamoylases. **Q. Wang**, J. Xia, V. Guallar, G. Krilov, E. R. Kantrowitz

**2:00 222.** Theoretical studies of uranyl complexes. **G. E. Schoendorff**, W. A. deJong, M. S. Gordon, T. L. Windus

**2:30 223.** Theoretical study on the interaction between xenon and positive silver clusters in the gas phase and on the (001) chabazite surface. **H. G. Nguyen**, G. Konya, E. M. Eyring, D. B. Hunter, T. N. Truong

**3:00** Intermission.

**3:10 224.** Interfacing the effective fragment potential with the reactive force field.

**S. A. Nedd**, M. S. Gordon

**3:40 225.** Using pseudo atoms to model silicon and silicon oxide surface chemistries with electronic structure theory. **H. P. Hratchian**, U. Das, G. A. Ferguson, K. Raghavachari

## ENVR

### Division of Environmental Chemistry

S. Al-Abed, *Program Chair*

#### OTHER SYMPOSIA OF INTEREST:

**Catalysis in Fuel Chemistry** (see *FUEL*, Mon, Tue, Wed, Thu)

**Coal Chemistry** (see *FUEL*, Wed)

**Emissions from Combustion Processes: Environmental Issues, Assessment, and Control** (see *FUEL*, Tue)

**Methods and Techniques in Analytical Characterization for Fuel Nanoscience** (see *FUEL*, Mon)

**Coprecipitation of Metals during Chemically and Biologically Induced Mineral Precipitation** (see *GEOC*, Sun, Tue)

**Geochemistry Division Award Symposium in honor of Fred T. Mackenzie** (see *GEOC*, Mon)

**Multiscale Reactions Including Fe-oxides, Oxyhydroxides, and Hydroxides** (see *GEOC*, Tue, Wed)

**Speciation and Kinetics in Natural Waters in Honor of Frank J. Millero** (see *GEOC*, Thu)

**Nanoscale Materials in Chemistry: Environmental Applications: In Honor of Professor Klabunde, I&EC Division Fellow** (see *I&EC*, Mon)

**Nanotechnology and the Environment: Emphasis on Green Nanotechnology** (see *I&EC*, Sun, Tue, Wed, Thu)

#### SOCIAL EVENTS:

Dinner: Tue

Social Hour: Tue

#### BUSINESS MEETINGS:

**Executive Committee Meeting:** Sun  
**Long Range Planning Subcommittee Meeting:** Sun  
**Program Planning Subcommittee Meeting:** Sun

### SUNDAY MORNING

Section A

Hilton  
Alpine Ballroom West

#### New Energy Technology Low Energy Nuclear Reactions: Introduction and Overview

J. Marwan, *Organizer, Presiding*

**8:30 1.** Introducing low energy nuclear reactions. **J. Marwan**

**8:55 2.** Low-energy nuclear reaction research: 2009 ACS update. **S. B. Krivit**

**9:20 3.** Condensed matter nuclear science discoveries. **S. R. Chubb Sr.**, T. A. Chubb

**9:45 4.** From cold fusion to condensed matter nuclear science: 20 years of research. **M. C. H. McKubre**

**10:10 5.** Twenty year history of LENR research using Pd/D codeposition.

**F. E. Gordon**, S. Szpak, P. A. Mosier-Boss, M. H. Miles, L. Forsley

**10:35 6.** From the proof of principle to a working prototype. **A. De Ninno**

**11:00 7.** Practical use of nuclear quadrupole and internal magnetic field augmented LENR. **D. Cravens**, R. Gimpel, V. Golubich

Please refrain from using cellular telephones and cameras during technical sessions.

‡ Cooperative Cosponsorship

## Section B

Hilton  
Canyon A**Geochemistry of Engineered Nanoparticles in the Environment** Cosponsored by NANOM. Chappell, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:35 8.** Influence of surface chemistry on the transport properties of multiwalled carbon nanotubes in porous media. **H. Fairbrother**, B. Smith, K. A. Wepasnick, W. P. Ball
- 8:55 9.** Formation and persistence of cadmium sulfide nanoparticles in aqueous solutions under various conditions. **K. M. Mullaugh**, J. M. Spraggins II, D. P. Ridge, G. W. Luther III
- 9:15 10.** Characterization of iron nanoparticles stabilized for enhanced delivery to TCE source zones. **B. M. Jung**, N. Sakulchaicharoen, D. M. O'Carroll, J. E. Herrera, B. E. Sleep
- 9:35 11.** Influence of natural organic matter on deposition rate of single-walled carbon nanotubes. **N. B. Saleh**, L. D. Pfefferle, M. Elimelech
- 9:55** Discussion and Intermission.
- 10:15 12.** Surfactive quality of humic substances for stabilizing carbon nanotube dispersions. **M. Chappell**, A. J. George, J. Mao, G. Bourne, C. L. Price
- 10:35 13.** Influence of cosolutes on the adsorption of Cd(II) onto oxidized multiwalled carbon nanotubes. **H.-H. Cho**, J. Yang, K. A. Wepasnick, H. Fairbrother, W. P. Ball
- 10:55 14.** Partitioning of nanoparticles in octanol and water. **K. D. Hristovski**, P. K. Westerhoff, **J. D. Posner**

**Detection and Monitoring of Engineered Nanoparticles in Environmental and Biological Systems** Sponsored by COLL, Cosponsored by ENVR<sup>+</sup> and NANO**Metal and Metalloid Speciation and Adsorption in Honor of James O. Leckie** Surface Complexation Modeling of Mineral Surfaces Sponsored by GEOC, Cosponsored by ENVR

## SUNDAY AFTERNOON

## Section A

Hilton  
Alpine Ballroom West**New Energy Technology**  
**Low Energy Nuclear Transmutation**J. Marwan, *Organizer, Presiding*

- 1:30 15.** Composition of particles in heavy water electrolyte after electrolysis. **J. Dash**, Q. Wang
- 1:55 16.** Transmutation with glow discharge. **I. B. Savvatimova**, J. Dash
- 2:20 17.** Reproducible generation of nuclear particles during electrolysis. **R. A. Oriani**
- 2:45 18.** Nuclear transmutation of isotopes in biological systems: History, models, experiments and perspectives. **V. Vysotskii**, A. Kornilova
- 3:10 19.** Nanonuclear reactions in condensed matter. **L. Forsley**, F. E. Gordon, P. A. Mosier-Boss
- 3:35 20.** Isotopic changes of elements caused by various conditions of electrolysis. **T. Mizuno**
- 4:00 21.** Characterization of distinctive materials with which to generate nuclear transmutation. **H. Kozima**

The official technical program for the 237th National Meeting is available online at [oasys2.confex.com/acs/237nm/techprogram/](http://oasys2.confex.com/acs/237nm/techprogram/).

- 4:25 22.** Effect of hydrogen stoichiometry (x) on the lattice expansion in metal-Hx systems. **N. Amanet**
- 4:50 23.** Understanding the palladium-hydrogen (deuterium) electrochemistry as crucial step to approach low energy nuclear reactions. **J. Marwan**

## Section B

Hilton  
Canyon A**Geochemistry of Engineered Nanoparticles in the Environment** Cosponsored by NANOM. Chappell, *Organizer, Presiding*

- 1:30 24.** Association of single-wall carbon nanotubes with natural particulate matter under estuarine conditions. **A. Schierz**, B. Englehart, A. Moore, P. L. Ferguson
- 1:50 25.** Development of heterogeneous catalyst capable of activating hydrogen peroxide at neutral pH values. **A. L. Pham**, C. Lee, F. M. Doyle, D. L. Sedlak
- 2:10 26.** EXAFS investigation of the oxidation and Fe-oxide speciation of Fe<sup>0</sup> nanoparticles (NZVI) under geochemically relevant conditions. **B. C. Reinsch**, C. S. Kim, G. V. Lowry
- 2:30 27.** Measuring sorption of metals to nanoparticles using flow field-flow-fractionation-inductively coupled plasma-mass spectrometry. **E. K. Lesher**, J. F. Ranville, B. D. Honeyman
- 2:50** Discussion and Intermission.
- 3:10 28.** Reactions of gas-phase naphthalene with paint and sunscreen surfaces containing TiO<sub>2</sub> nanoparticles. **N. Ashley**, N. McBride, J. Krumholtz, B. Baker, K. T. Valsaraj
- 3:30 29.** Uranium(VI) removal by nanoscale zerovalent iron under anoxic conditions. **S. Yan**, Z. Bao, B. Deng

**Detection and Monitoring of Engineered Nanoparticles in Environmental and Biological Systems** Sponsored by COLL, Cosponsored by ENVR<sup>+</sup> and NANO**Metal and Metalloid Speciation and Adsorption in Honor of James O. Leckie** Mineral Surface Speciation Sponsored by GEOC, Cosponsored by ENVR

## MONDAY MORNING

## Section A

Hilton  
Alpine Ballroom West**New Energy Technology**  
**Tritium, Neutron Production and Bubble Fusion**J. Marwan, *Organizer, Presiding*

- 8:30 30.** Characterization of neutrons emitted during Pd/D co-deposition. **P. A. Mosier-Boss**, S. Szpak, F. E. Gordon, L. Forsley
- 8:55 31.** Field-assisted electroplating. **J. A. Yurkovic**, S. J. Zaksorn, N. D. Robertson, H. Saito
- 9:20 32.** Anomalous tritium production in CMNS. **X. Z. Li**
- 9:45 33.** Advances in acoustic inertial confinement bubble nuclear fusion. **R. C. Block**, R. T. Lahey, R. I. Nigmatulin, **R. P. Taleyarkhan**
- 10:10 34.** When bubble cavitation becomes sonofusion. **R. S. Stringham**
- 10:35 35.** Observation of high multiplicity neutron emission events from deuterated Pd and Ti samples at BARC: A review. **M. Srinivasan**
- 11:00 36.** Observation of neutrons and tritium in a wide variety of LENR configurations: BARC results revisited. **M. Srinivasan**
- 11:25 37.** Discovery of Erzion nuclear reaction tracks in the space. **Y. N. Bazhutov**

## Section B

Hilton  
Canyon A**Frontiers in Water Reuse: Detection, Advanced Treatment and Environmental Fate of Contaminants of Emerging Concern**  
**Analytical Methods and Occurrence**E. P. Kolodziej and D. M. Cwiertny, *Organizers, Presiding*

- 8:30** Introductory Remarks.
- 8:40 38.** Hormones, pharmaceuticals, and other trace wastewater derived contaminants: Detection, fate, and environmental effects. **J. L. Gray**, A. M. Vajda, L. B. Barber, E. T. Furlong, W. T. Foreman, V. Blazer, D. W. Kolpin, D. O. Norris
- 9:20 39.** Passive sampler with direct spectral detection for rapid screening of waters for emerging contaminants. **T. C. G. Kibbey**, L. Chen, D. A. Sabatini
- 9:40 40.** Determination of pharmaceuticals identified as emerging pollutants by capillary electrophoresis with capacitively coupled contactless conductivity detection. **S. F. Y. Li**
- 10:00** Intermission.
- 10:20 41.** Endocrine disrupting chemicals and other emerging contaminants in wastewater and drinking water treatment technologies. **M. Mills**
- 11:00 42.** Macro- vs. micropollutants in impaired waters: What really matters? **W. A. Mitch**, S. S. Walse
- 11:20 43.** Evaluation of functional groups responsible for chloroform formation during water chlorination using compound specific isotope analysis. **W. A. Arnold**, J. Bolotin, U. von Gunten, T. B. Hofstetter

**Metal and Metalloid Speciation and Adsorption in Honor of James O. Leckie** Applications of Adsorption Models Sponsored by GEOC, Cosponsored by ENVR**Redox Biogeochemistry of Phyllosilicate Minerals** Sponsored by GEOC, Cosponsored by ENVR

## MONDAY AFTERNOON

## Section A

Hilton  
Alpine Ballroom West**New Energy Technology**  
**Excess Heat Production**J. Marwan, *Organizer, Presiding*

- 1:30 44.** Reports of anomalous self-heating events. **S. B. Krivit**
- 1:55 45.** Twenty year review of isoperibolic calorimetric measurements of the Fleischmann-Pons effect. **M. H. Miles**, M. Fleischmann
- 2:20 46.** "Hot" deuteron generation and charged particle emission during excitation of the deuteron subsystem in metal deuterides. **A. G. Lipson**, I. P. Chernov, A. S. Roussetski, A. Y. Tsvadze, B. F. Lyakhov, Y. P. Cherdantsev, M. E. Melich, E. I. Saunin
- 2:45 47.** Gas-loading experiments for self-sustaining heat in CMNS. **X. Z. Li**
- 3:10 48.** Excess heat and electrical characteristics of type "B" anode-plate at low energy nuclear reactions. **M. Swartz**
- 3:35 49.** Anomalous heat generation during hydrogenation of carbon hydride. **T. Mizuno**
- 4:00 50.** Dual laser stimulation of optical phonons in palladium deuteride. D. Letts, **D. Cravens**, P. L. Hagelstein
- 4:25 51.** Deuterium gas charging experiments with Pd powders for excess heat evolution. A. Kitamura, T. Nohmi, Y. Sasaki, T. Yamaguchi, A. Taniike, **A. Takahashi**, R. Seto, Y. Fujita

## Section B

Hilton  
Canyon A**Frontiers in Water Reuse: Detection, Advanced Treatment and Environmental Fate of Contaminants of Emerging Concern**  
**Fate in the Natural Environment and Conventional Treatment Systems**E. P. Kolodziej and D. M. Cwiertny, *Organizers, Presiding*

- 1:30 52.** Water reuse for ecosystem support. **M. Reinhard**
- 2:10 53.** Antibiotics at environmental interfaces studied by nonlinear optics. **F. M. Geiger**, P. L. Hayes
- 2:30 54.** Factors controlling the adsorption on effluent-derived pharmaceuticals on mineral surfaces. **D. M. Cwiertny**, S. Qu
- 2:50 55.** Mechanism for adsorption of Lincomycin from water by clay minerals. **C. Wang**, J. Y. Ding, B. J. Teppen, S. A. Boyd, H. Li
- 3:10** Intermission.
- 3:30 56.** Elucidating the fate of ultraviolet filter chemicals in the aquatic environment. J. Klein, M. Wu, M. L. Tse, **L. A. MacManus-Spencer**
- 3:50 57.** Reactivity of bisphenol-A with free chlorine in the presence of iodide and bromide. **E. M. Fiss**, **P. J. Vikesland**
- 4:10 58.** Removal of pharmaceutical pollutants via solar photolysis and sludge digestion. **C. C. Ryan**, D. Diehl, W. A. Arnold
- 4:30 59.** Comparison of estrogen degradation under various wastewater treatment schemes. **L. Racz**, R. Goel

**Undergraduate Research Poster Session: Environmental Chemistry** Sponsored by CHED, Cosponsored by ENVR and SOCED

## MONDAY EVENING

## Section A

Salt Palace Convention Center  
Hall 5

## Sci-Mix

S. R. Al-Abed, *Organizer*

## 8:00-10:00

**128, 130, 133, 135-136, 139-140, 142, 146-147, 149, 151, 155, 159, 162, 164, 169-170, 172, 187, 193, 199.** See subsequent listings.

## TUESDAY MORNING

## Section A

Hilton  
Alpine Ballroom West**New Energy Technology**  
**Low Energy Nuclear Reactions:**  
**Theoretical Approach**J. Marwan, *Organizer, Presiding*

- 8:30 60.** Energetics of condensed matter cluster reactions in nanostructured palladium. **G. H. Miley**, X. Yang, N. Luo, H. Hora
- 8:55 61.** Withdrawn.
- 9:20 62.** Overcoming the Coulomb barrier and related effects through resonant electromagnetic dynamics and quantum mechanics in the Fleischmann-Pons effect. **S. R. Chubb Sr.**
- 9:45 63.** Simulating anomalies in metal deuterides. **P. L. Hagelstein**, I. U. Chaudhary
- 10:10 64.** Understanding low energy nuclear reactions. **A. De Ninno**
- 10:35 65.** Basics of deuteron-cluster dynamics by Langevin equation. **A. Takahashi**
- 11:00 66.** Cold nuclear fusion mechanism at crack tip spearhead located deep under the ground. **A. V. Shestopalov**

## Section B

Hilton  
Canyon A**Frontiers in Water Reuse: Detection, Advanced Treatment and Environmental Fate of Contaminants of Emerging Concern  
Advanced Treatment Technologies**E. P. Kolodziej and D. M. Cwiertny,  
*Organizers, Presiding*

- 8:30** Introductory Remarks.
- 8:40 67.** Oxidation of bulk and trace organics in reverse osmosis concentrate.  
**P. K. Westerhoff**
- 9:20 68.** Oxidation of N-nitrosodimethylamine (NDMA) using boron-doped diamond film electrodes. **B. P. Chaplin**, C. Duncan, G. Schrader, J. Farrell
- 9:40 69.** Detoxification of water contaminated with the cyanotoxin, microcystin-LR, by utilizing thin TiO<sub>2</sub> photocatalytic films.  
**M. G. Antoniou**, P. A. Nicolaou, A. A. de la Cruz, D. D. Dionysiou
- 10:00 70.** Removal of acetaminophen in enzyme-mediated oxidative coupling process: Reaction rates and pathways.  
**J. Lu**, Q. Huang
- 10:20** Intermission.
- 10:40 71.** Withdrawn.
- 11:20 72.** Novel osmotically driven hybrid process for potable reuse of impaired water. **T. Y. Cath**, J. Drewes, C. Lundin
- 11:40 73.** Water treatment using hybrid ozonation-membrane filtration.  
**S. H. R. Davies**, A. L. Alpatova, M. J. Baumann, L. M. Cornell, J. Kim, V. V. Tarabara, S. J. Masten

## Section C

Hilton  
Salon II**Exposure of Engineered Nanomaterials**  
Cosponsored by NANON. F. Savage, *Organizer*

- 9:00** Introductory Remarks.
- 9:10 74.** Aggregation kinetics of carbon nanotubes in the presence of biomacromolecules. **N. B. Saleh**, L. D. Pfeifferle, M. Elimelech
- 9:35 75.** Bacterial toxicity of carbon-based nanomaterials: Implication for natural and engineered aquatic system. **S. Kang**, M. S. Mauter, M. Elimelech
- 10:00 76.** Behavior of natural and laboratory prepared metal oxyhydroxides in a constructed wetland system receiving acid mine drainage. **B. N. Gartman**, J. F. Ranville
- 10:25** Intermission.
- 10:40 77.** Detection of nanosilver and fullerenes in several commercial products.  
**P. K. Westerhoff**, T. M. Benn, B. Cavanagh
- 11:05 78.** Effects of pH and hardness on the environmental stability of ZnS and CdS nanoparticles. B-T. Lee, A. Striz,  
**J. F. Ranville**

**Food-related Nanotechnology Application and Characterization**  
Sponsored by AGFD, Cosponsored by ENVR and NANO**Metal and Metalloid Speciation and Adsorption in Honor of James O. Leckie**

**Photographing or recording meeting sessions and/or activities other than your own are prohibited at all official ACS events without written consent from ACS.**

**Reactivity of Carbonates, Sulfides, and other Minerals** Sponsored by GEOC, Cosponsored by ENVR

## TUESDAY AFTERNOON

## Section A

Hilton  
Alpine Ballroom West**New Energy Technology General**J. Marwan, *Organizer, Presiding*

- 1:00 80.** Physical model and direct experimental observation of water memory and biophysical activity of magnetic-activated water. **V. Vysotskii**, A. Kornilova
- 1:25 81.** Kinetics in a unique sodium borohydride regenerative fuel cell. **G. H. Miley**, N. Luo, X. Yang, K-J. Kim, G. Kopec
- 1:50 82.** Catching CO<sub>2</sub> in a bowl.  
**J. A. Tossell**
- 2:15 83.** Photoelectrochemical characterization of semiconductor materials for solar water splitting. **T. G. Deutsch**, J. A. Turner

## Section A

Hilton  
Alpine Ballroom West**ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences: Symposium in Honor of Shirley McBay** Cosponsored by CMA, CPS, and WCCR. A. Hathaway, *Organizer*M. G. Rosenthal, *Presiding*

- 3:30 79. Award Address** (ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences, sponsored by The Camille and Henry Dreyfus Foundation, Inc). Environmental justice: A leadership role for environmental chemists.  
**S. McBay**

## Section B

Hilton  
Canyon A**Frontiers in Water Reuse: Detection, Advanced Treatment and Environmental Fate of Contaminants of Emerging Concern  
Advanced Treatment Technologies**E. P. Kolodziej and D. M. Cwiertny,  
*Organizers, Presiding*

- 1:30 84.** Advanced treatment technologies for removal of pathogens and chemical pollutants for water reuse. **K. G. Linden**
- 2:10 85.** Removing beta-lactam antibiotics from contaminated waters using radical reactions. **M. K. Dail**, S. P. Mezyk, J. R. Peller
- 2:30 86.** AO/OP radical chemistry of mixed aliphatic-aromatic nitrosamines in water.  
**E. Abud**, S. P. Mezyk, K. L. Swancutt, T. Foust, J. J. Kiddle
- 2:50 87.** Sonolytic degradation of aqueous film forming foams (AFFFs). **C. D. Vecitis**, Y-J. Wang, J. Cheng, B. Mader, M. R. Hoffmann
- 3:10** Intermission.
- 3:30 88.** Advances in the treatment of wastewater-derived micropollutants with permanganate and ferrate oxidizing agents.  
**T. J. Strathmann**, L. Hu, H. M. Martin
- 4:10 89.** Aqueous electron reduction of fluorochemicals. **C. D. Vecitis**, H. Park, B. Mader, M. R. Hoffmann
- 4:30 90.** Absolute kinetics and efficiencies of hydroxyl radical and hydrated electron reactions with sulfa drugs in water.  
**T. Neubauer**, S. P. Mezyk, W. J. Cooper, J. R. Peller
- 4:50 91.** Absolute rate constant measurements for the hydroxyl radical ( $\cdot\text{OH}$ ) with effluent organic matter. **D. F. R. Doud**, S. P. Mezyk, F. Rosario-Ortiz

## Section C

Hilton  
Salon II**Exposure of Engineered Nanomaterials**  
Cosponsored by NANON. F. Savage, *Organizer*

- 1:30 92.** Extraction of fullerene (nano-C<sub>60</sub>) from artificial sediment. **J. Wang**, Q. Cai, T. A. Anderson, G. P. Cobb III
- 1:55 93.** Fe<sup>0</sup> nanoparticles remain mobile in porous media after eight months aging due to slow desorption of polymeric surface modifiers. **H-J. Kim**, T. Phenrat, R. D. Tilton, G. V. Lowry
- 2:20 94.** Microbiological fate of nanoparticles commonly found in personal care products. **C. L. Gruden**, O. Mileyeva-Biebesheimer
- 2:45** Intermission.
- 3:00 95.** Safe handling and disposal of nanomaterials: Lessons from and challenges for exposure research.  
**H. A. Godwin**, E. Suarez
- 3:25 96.** Uptake and depuration of nanoscale titanium dioxide particles (nTiO<sub>2</sub>) by *Daphnia* and zebrafish. **X. Zhu**, Y. Chang, Y. Chen
- 3:50** Concluding Remarks.

**Food-related Nanotechnology Nanoencapsulation and Nanoemulsions**  
Sponsored by AGFD, Cosponsored by ENVR and NANO**Metal and Metalloid Speciation and Adsorption in Honor of James O. Leckie Heterogeneous Redox Reactions**  
Sponsored by GEOC, Cosponsored by ENVR

## TUESDAY EVENING

**Geochemical Processes, Reactivity, and Applications of Manganese Oxides**  
Sponsored by GEOC, Cosponsored by ENVR and INOR**Metal and Metalloid Speciation and Adsorption in Honor of James O. Leckie**  
Sponsored by GEOC, Cosponsored by ENVR

## WEDNESDAY MORNING

## Section A

Hilton  
Alpine Ballroom West**Evaluation of the Sustainability of Drinking Water Technologies: Application in the Developing World** Cosponsored by AEEPSC. J. Clark and A. Lindner, *Organizers*A. T. Cooper, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:35 97.** Reduction of perchlorate from contaminated waters using zero valent iron and palladium enhanced by UV light.  
**A. Q. Zhao**, E. Sahle-Demessie, G. A. Sorial
- 9:00 98.** Removing bacteria and heavy metals from drinking water with cactus mucilage. **A. Buttice**, D. I. Fox, T. Pichler, J. Stroot, D. V. Lim, D. H. Yeh, P. Stroot,  
**N. Alcantar**
- 9:25 99.** Studies on the removal of nitrate from water by Ca/Al chloride hydrotalcite-like compound. **R. Patel**
- 9:50** Intermission.
- 10:05 100.** Experiences in southern India.  
**M. D. Guroi**, C. Sirin
- 10:30 101.** The best option? Drinking water treatment or advances in supply and storage. **J. R. Mihelcic**, M. A. Troitz, E. Omisca
- 10:55** Concluding Remarks.

‡ Cooperative Cosponsorship

## Section B

Hilton  
Canyon A**Environmental Toxicology From Paracelsus to Probabilistic Risk Assessment**U. Friederich, *Organizer*G. P. Cobb III, *Organizer, Presiding*

- 8:30 102.** Assessing exposures to pesticides. **J. N. Seiber**, R. I. Krieger, J. E. Woodrow
- 8:50 103.** Pharmaceuticals in fish: Perspectives of an analytical chemist.  
**P. Perez-Hurtado**, A. J. Ramirez, B. W. Brooks, **C. K. Chambliss**
- 9:10 104.** RDX fate in saturated surface sediments: Biological transformation and plant uptake. **A. Jackson**, S. Sanka, D. Low, T. A. Anderson
- 9:30 105.** Occurrence and potential toxicity of pyrethroids and other insecticides in bed sediments of urban streams in central Texas. **J. Belden**, E. Hintzen, M. J. Lydy
- 9:50 106.** Toxicity testing: Integration of potential chemicals of concern using bioavailability. **W. L. Goodfellow Jr.**, J. C. Baummer III, W. L. McCulloch, M. C. Ciarlo, R. J. Neubauer
- 10:10 107.** Environmental impacts and biogeochemical evaluation of stormwater retention ponds: Red Run watershed, MD case study. **D. R. Ownby**, R. E. Casey, S. M. Lev, J. W. Snodgrass

**Food-related Nanotechnology Health and Safety** Sponsored by AGFD, Cosponsored by ENVR and NANO**Metal and Metalloid Speciation and Adsorption in Honor of James O. Leckie Speciation and Microbial Systems**  
Sponsored by GEOC, Cosponsored by ENVR

## WEDNESDAY AFTERNOON

## Section A

Hilton  
Alpine Ballroom West**Environmental Distribution, Degradation, and Mobility of Explosives and Propellant Compounds**M. Chappell, *Organizer, Presiding*

- 1:30** Introductory Remarks.
- 1:40 108.** Assessing sample processing and sampling uncertainty for energetic residues on military training ranges: Method 8330B.  
**A. D. Hewitt**, M. Walsh, M. R. Walsh, S. Bigl, M. Chappell
- 2:00 109.** Predicting releases of munition constituents from breached shells in the marine environment. **P-F. Wang**, Q. Liao, R. George, W. Wild
- 2:20 110.** Optimization of TNT partitioning coefficient (K<sub>d</sub>) in marine sediments.  
**M. Chappell**, C. L. Price, B. E. Porter, G. Bourne, L. Ford, A. J. George
- 2:40 111.** TNT, RDX, and HMX association with organic fractions of marine sediments and bioavailability implications.  
**J. C. Pennington**, G. R. Lotufo, C. Hayes, B. Porter, **R. George**
- 3:00** Discussion.
- 3:15 112.** Environmental hazard and distribution resulting from explosives contamination and high pressure liquid and gas chromatography/mass spectroscopic analogs. **T. D. Adepoju**, R. C. Nwokoma, **N. R. Nwokoma**
- 3:35 113.** Using compound-specific carbon and nitrogen isotope analysis for the assessment of nitroaromatic compound transformation. **T. B. Hofstetter**, A. E. Hartenbach, J. C. Spain, S. F. Nishino, R. P. Schwarzenbach
- 3:55 114.** Use of Raman/SERS to evaluate chemistries for the detection and/or remediation of perchlorate in aqueous systems.  
**P. A. Mosier-Boss**

4:15 **115.** Decontamination of TNT, RDX, and HMX explosive wastewaters using zero-valent iron nanoparticles. **K-S. Lin**, K-Y. Li, S-F. Jeng, M-J. Hsien

#### Section B

Hilton  
Canyon A

#### Environmental Toxicology Emerging Issues

U. Friederich, *Organizer*

G. P. Cobb III, *Organizer, Presiding*

- 1:30 **116.** Bioaccumulation of radioactively labeled multiwalled carbon nanotubes by *Daphnia magna*. **E. J. Petersen**, J. Akkanen, J. Kukkonen, W. J. Weber Jr.
- 1:50 **117.** Nanoparticle adhesion leads to impaired locomotor function and mortality in adult *Drosophila*. **D. Vinson**, X. Liu, D. Rand, R. H. Hurt
- 2:10 **118.** Nanoparticle CuO displays significant cytotoxicity: Implication for oxidative stress. **X. Pan**, K. Yarlagadda, K. P. Gidda, J. S. McConnell, B. Zhang
- 2:30 **119.** Withdrawn.

#### Section C

Hilton  
Salon II

#### Evaluation of the Sustainability of Drinking Water Technologies: Application in the Developed World

Cosponsored by AEEESP

A. T. Cooper and A. Lindner, *Organizers*

C. J. Clark, *Organizer, Presiding*

- 1:30 **Introductory Remarks.**
- 1:35 **120.** Influence of water chemistry on the stability of lead-containing phases present in drinking water distribution systems. **D. E. Giammar**, K. Nelson, J. D. Noel, Y. Xie
- 1:55 **121.** Isolation of natural organic matter in source water and characterization of trihalomethanes precursors by fluorescence spectroscopy. **K. Punburananon**, T. F. Marhaba
- 2:15 **122.** Determination of disinfection by-products formation using multivariate statistical analysis of fluorescence spectra. **K. Punburananon**, T. F. Marhaba
- 2:35 **123.** Innovative approach for treating oxidant-laden residual streams. **J. Brown**, R. D. Wheadon, C. Christiansen, E. J. Hansen
- 2:55 **Intermission.**
- 3:10 **124.** Treatment of reverse osmosis concentrate to improve overall recovery: Parameter effects on antiscalant oxidation and subsequent precipitation. **L. F. Greenlee**, B. Marrot, P. Moulin, B. D. Freeman, D. F. Lawler
- 3:30 **125.** Evaluation of nanoscale zero-valent iron in drinking water technology: Degradation of bromate in water treatment. **Q. Wang**, S. A. Snyder, H. Choi
- 3:50 **126.** Colorimetric-solid phase extraction (C-SPSE) for the determination of trace level indicators of water quality. **L. M. Siperko**, M. D. Porter, R. J. Lipert
- 4:10 **Concluding Remarks.**

#### Metal and Metalloid Speciation and Adsorption in Honor of James O. Leckie

**Environmental Sciences, Engineering, and  
Dermal Exposure** Sponsored by GEOC,  
Cosponsored by ENVR

#### WEDNESDAY EVENING

#### Section A

Salt Palace Convention Center  
Hall 5

#### General Papers

S. R. Al-Abed, *Organizer, Presiding*

#### 6:00-8:00

127. Biodistribution and toxicity of systemically-introduced ceria engineered nanomaterial. **R. A. Yokel**, R. L. Florence, J. M. Unrine, M. T. Tseng, U. M. Graham, R. Sultana, D. A. Butterfield, P. Wu, E. Gulke
128. Evaluating the impact of varying synthesis methods on surface charging and aggregation of silver nanoparticles. **A. El-Badawy**, **T. Luxton**, T. Tolyamat, K. G. Scheckel
129. Silver speciation and leachability from silver nanomaterial containing consumer fabric. **A. El-Badawy**, **T. Luxton**, K. Scheckel, T. Tolaymat, M. Suidan
130. Studying the interaction of particulate matter with biological media. **D. Berube**, X. Liao, T. Yapici
131. Synthesis of a novel Schiff base ethane-1,2-diy(dibis)nitrobenzylidene ethane-1,2-diamine as an ionophore for sulfate selective electrode. **A. Sathyapalan**, A. Zhou
132. Synthesis of nanohydroxyapatite and its application for uranium remediation. **S. R. Kanel**, M. O. Barnett, T. P. Clement
133. Effects of atrazine on dimethyl sulfur metabolism of marine phytoplankton. **C. E. Spiese**, D. J. Kieber
134. Effects of unknown source on the colinearity problem in CMB model. **G. Shi**, **X. Li**, T. Wu, Y-C. Feng, X-H. Bi, J-H. Wu, T. Zhu
135. Unsteady-state chemodynamic fate and transport model for in-home pollutants following Hurricane Katrina. **N. Ashley**, K. T. Valsaraj, L. Thibodeaux
136. Use of poly(4-vinylpyridine) for removal of perchlorate from aqueous solution through polyelectrolyte enhanced ultrafiltration. **J. D. Roach**, R. F. Lane
137. Utilization of steam to recover the caustic and alumina from red mud slurry. **R. Patel**
138. Water uptake of humic and fulvic acid: Aerosol and thin film measurements. **C. D. Hatch**, K. M. Gierlus, J. Zahardis, J. D. Schuttelfield, V. H. Grassian
139. Preliminary study on immobilization of heavy metals in municipal solid waste incineration fly ash with geopolymer. **M. Jin**, Q. Zhang, **L. Wang**
140. Raw humics extract and military smoke dye as extracellular electron shuttles. **M. J. Kwon**, B. Powers, K. T. Finneran
141. Reactive activated carbon impregnated with Fe/Pd: PCBs dechlorination reactivity and capacity, aging, and oxidation. **H. Choi**, S. R. Al-Abed, S. Agarwal, E. Graybill
142. Recycling of plasma-melted slags utilized in TIMS. **H-L. Huang**
143. Reductive degradation of personal care products using zero-valent metals. **Y-H. Kim**, S-O. Ko, M-C. Kim, J. H. Kim, H. S. Oh
144. Seasonal variation of atmospheric CH<sub>4</sub>, N<sub>2</sub>O and CO<sub>2</sub> and causes analysis in Tianjin offshore area of Bohai Sea. **S. Kong**, B. Han, **Z. Bai**, Z. Xu, C. Wu, B. Zhang
145. Selective adsorption of heavy metals onto porous materials. **Y. H. Kim**, W. S. Shin, S. J. Choi, I. Hwang, J-H. Choi, W. T. Lim, H. S. Oh, W. S. Jang
146. Software tools facilitating QSPR studies of congeneric sets of organic pollutants. **M. Haranczyk**, T. Puzyn
147. Soil transport and microbial impact of magnetite nanoparticles. **K. F. Starr**, Q. Liang, Y. Feng, **D. Zhao**
148. Sorption of lead and cadmium from aqueous solutions by *Nasturtium officinale*. **V. Alicea-Vázquez**, M. Romero-Perez, M. Ramos-Fontán, J. Arbelo-García

149. Bioaccumulation and toxicity of silver nanoparticles in animal and plant tissues. **I. E. Pavel**, **J. Monahan**, M. M. Markopoulos, Z. E. Gagnon, B. NeJame
150. Photoformation of hydroxyl radical from water-soluble organic matter in atmospheric aerosol. **H. Kondo**, K. Takeda, H. Sakugawa
151. Sorption of ultraviolet filter chemicals to sediment. **M. Wu**, L. A. MacManus-Spencer
152. Withdrawn.
153. PAH concentrations in PM<sub>2.5</sub> generated during prescribed burns of the Coconino and Apache-Sitgreaves National Forests. **M. S. Robinson**, P. Herckes, L. Portz
154. Paraoxon-induced acute brain dysfunction: Increase of EEG (electroencephalography)  $\delta$  power spectra in rats. **Z. Gu**, R. A. Bauman, J. B. Long
155. Withdrawn.
156. Photocatalytic degradation of trichloroethylene on zinc oxide nanorods. **T-F. Hsu**, T-L. Hsiung, Y-L. Wei, **H. P. Wang**
157. Photochemical degradation of ultraviolet filter chemicals in surface waters. **J. Klein**, M. L. Tse, L. A. MacManus-Spencer
158. Improved understanding of Pd/Mg systems through a study of critical system parameters. **S. Agarwal**, S. R. Al-Abed, D. D. Dionysiou
159. Influence of environmental temperature and relative humidity on photocatalytic oxidation of toluene adsorbed on activated carbon fibers coated TiO<sub>2</sub>. **C. Wu**, T. Guo, Z. Bai, **T. Zhu**, **X. Li**, **M. Dai**, **S. Peng**
160. Influence of relative humidity on the photocatalytic oxidation (PCO) of toluene by TiO<sub>2</sub> loaded on activated carbon fibers: PCO rate and intermediates accumulation. **T. Guo**, **C. Wu**, Z. Bai, T. Zhu, **X. Li**, **M. Dai**, **S. Peng**
161. Measurement of criteria air pollutants in a residential area of Kuwait. **K. N. Jallad**
162. Mixed metal oxide nanocomposites: Novel extractants for the remediation of arsenate from aqueous solutions. **T. M. Trad**, M. Chehbouni
163. Element characteristic of atmospheric PM<sub>10</sub> and source identification based on qualitative methods in Teda, Tianjin. **S. Kong**, B. Han, Z. Bai, Z. Xu, X. Li, B. Zhang
164. Effect of functional groups in dispersants for the transport of titanium dioxide nanoparticles in quartz sands. **S. H. Joo**, T. Luxton, S. R. Al-Abed
165. Extraction of toxic metal ions with nanosize hollow carbon spheres. **C-K. Tsai**, C-H. Huang, T-L. Hsiung, C-J. G. Chou, **H. P. Wang**
166. Fecal coliform source identification using chemical tracers. **N. Fahrenfeld**, A. Elzerman, J. T. Coates
167. Host-guest interactions of cyclodextrins and cyanotoxins. **L. Chen**, K. E. O'Shea
168. Immobilization of heavy metals using slag and phosphates. **F. Li**, **W. S. Shin**, I. Hwang
169. Dechlorination of trichloroethylene (TCE) using zero-valent iron in organic solvents. **R. E. Cook**, K. A. Thoreson, K. McNeill
170. Distribution and characteristics of PAHs in sediments from the coastal environment of Egypt. A. Mostafa, T. L. Wade, S. T. Sweet, N. B. El Sayed, **A. O. Barakat**
171. Effects of endosulfan on soil respiration. **R. Joseph**, S. T. Reed, C. S. Clark-Cuadrado, K. Jayachandran

172. Electrochemical oxidation of 4-chlorophenol with granular graphite electrodes. **J-L. Chen**, G. C. Chiou, C-C. Wu, K-Y. Chiang
173. Withdrawn.
174. Chelating polymers for removal of Pb on ppb levels: Capacity and kinetic studies. **P. Amoyaw**, C. W. Ingram, **X. R. Bu**
175. Chlorine-free disinfection of water contaminated with *Salmonella typhimurium* by treatment with an alternating current: Role of hydroxyl radicals formation. **N. N. Barashkov**, D. Eisenberg, S. Eisenberg, L. Lam, T. S. Novikova, G. S. Shegebaeva, I. S. Irgibaeva
176. Cloud point extraction for the detection of radionuclides in water samples. **S. Pepper**, D. R. Peterman, T. J. Tranter
177. Contaminant diffusion and degradation studies with alginate encapsulated iron nanoparticles. **R. Y. Shabnam**, S. Simsek, J. M. Thompson, E. Khan, A. Bezbaruah
178. Continuous flow fixed-bed biodiesel production from algae oil. **B. Wen**, J. P. Zhang, G. Wen
179. Correlation of the common water quality parameters pH, nitrate, phosphate, iron, total carbonate, and natural organic matter with the multifactorial photodegradation of *N*-octanoyl-DL-homoserine lactone. **R. L. Frey**, A. Decho, J. L. Ferry
180. Effect of temperature on the performance and biomass characteristics in EBPR system. **N. Li**, X. Wang, N. Ren, H. Kang, K. Zhang
181. Withdrawn.
182. Withdrawn.
183. Assessment of phytoavailability of arsenate in soils using the iron oxide-impregnated filter paper extraction method. **W-C. Kuo**, T-H. Lin, **D-Y. Lee**
184. Black carbons dominate sorption and desorption of polycyclic aromatic hydrocarbon onto lake sediments. **Q. Wu**, W. S. Shin
185. Cadmium accumulation and distribution in pak choi (*Brassica chinensis*) cultivated in the peri-urban areas of Hangzhou city, China: Implications for human health. **S. Yan**, Q. Ling, Z. Bao, Z. Chen, S. Yan, Z. Dong, B. Zhang
186. Catalytic reduction of nitrate with bimetallic iron nanoparticles. **H. Kang**, **Z. Xiu**, L. Li, Z. Jin, Z. Yang
187. Changes in water quality and prediction of acidity decay in 40 above drainage mines in West Virginia. **J. G. Skousen**, B. Mack
188. Characterization of elements in ambient particulate matter collected in Tianjin offshore area of Bohai Sea in summer and its source apportionment. **B. Han**, **S. Kong**, Z. Bai, Z. Xu, X. Li, B. Zhang
189. Characterization of residual nonaqueous phase liquids in different fractional wettability porous media. **R. I. Al-Raoush**
190. Application of green waste biochar for removal of pesticide residues. **W. Zheng**, M. Guo, N. Rajagopalan, T. Chow
191. Arsenic and heavy metals survey of rural ground waters in Nigeria. **E. Inam**, G. Ebong, K-W. Kim
192. Adsorption of heavy metals (zinc, cadmium and lead) which are commonly present in our atmosphere (Nigeria), and Western world using tigemutx' chaff (*Cyperus esculentus*), carboxymethylation and thioline modification processes. **C. P. Nwokoma**, **C. E. Ubani**, N. C. P. Nwokoma, **C. R. Nwokoma**
193. Adsorptive removal of cobalt, strontium and cesium using AMP-PAN in laundry wastewater from nuclear power plant. **Y-J. Park**, Y-C. Lee, W. S. Shin, S-J. Choi
194. Advanced treatment and targeted remediation of chlorinated compounds using supported nanoscale zerovalent iron. **V. T. John**, Y. Lu, J. Zhan, B. Sunkara, G. Pringer, G. McPherson

The official technical program for the 237th National Meeting is available online at [oasys2.confex.com/acs/237/nm/techprogram/](https://oasys2.confex.com/acs/237/nm/techprogram/).

195. Aldehyde emission measurements from ethanol fueled passenger vehicle.  
**H. Yamada**, K. Suzuki, T. Sakamoto, Y. Goto
196. Experimental study on the algae removal by microwave irradiation. **Q. Xie**
197. Deeper insight to Hg bioaccumulation in the bat population in Kentucky and Tennessee. **L. Clark**, E. Whitehouse, C. Webb
198. New method for high-throughput perchlorate analysis. **K. H. Kucharzyk**, R. Crawford, A. J. Paszczynski, T. F. Hess
199. *A priori* prediction of Hg(II) complexation by natural organic matter. **A. Mousavi**, S. E. Cabaniss
200. Adsorption of  $\text{Co}^{2+}$ ,  $\text{Sr}^{2+}$  and  $\text{Cs}^+$  on phosphate-modified montmorillonite.  
**B. Ma**, W. S. Shin, Y. H. Kim, S. J. Choi
201. Experiment research of attapulgite clay on its modification and the removal of nitrogen and phosphorus. **W. Chundu**, L. Churxia, X. Qingjie

## Section B

Salt Palace Convention Center  
Hall 5

### Geochemistry of Engineered Nanoparticles in the Environment

Cosponsored by NANO

M. Chappell, *Organizer, Presiding*

## 6:00–8:00

202. Preparation and characterization of a magnetic nanosized polyaluminum and its application in wastewater treatment.  
**W. Chundu**, L. Xing, X. Qingjie
203. Oxidation of zero-valent iron nanoparticles: Implications for reactivity and opportunities for regeneration. **Y. Xie**, D. M. Cwierny

## Section C

Salt Palace Convention Center  
Hall 5

### Exposure of Engineered Nanomaterials

Cosponsored by NANO

N. F. Savage, *Organizer*

## 6:00–8:00

204. Investigation of photochemical properties of  $\text{C}_{60}$  aggregates in water. **L. Kong**, K. Chen, R. Zepf

## Section D

Salt Palace Convention Center  
Hall 5

### Nanotoxicology: Ecotoxicity of Manufactured Nanomaterials

Cosponsored by NANO

N. F. Savage and S. R. Al-Abed,  
*Organizers*

## 6:00–8:00

205. Cytotoxicity study of nanoengineered  $\text{C}_{60}$  colloidal suspensions. **S. Kuriyavar**, Y. Zhang, J. Damron, R. Maples, B. Muriadanti, M. Hilburn, C. Pope, K. Ausman
206. Cellular uptake and cytotoxicity of gold nanorods: Molecular origin of cytotoxicity and surface effects. **A. M. Alkilany**, P. K. Nagaria, C. J. Murphy, C. R. Hexel, T. J. Shaw, M. D. Wyatt

**Please refrain from using cellular telephones and cameras during technical sessions.**

## Section E

Salt Palace Convention Center  
Hall 5

### Environmental Distribution, Degradation, and Mobility of Explosives and Propellant Compounds

M. Chappell, *Organizer, Presiding*

## 6:00–8:00

207. Canadian approach to the environmental characterization and risk assessment of military training activities. **S. Brochu**, R. Martel, G. Comeau, V. Nadeau, A. D. Hewitt
208. Environmental assessment of small arms live firing: Study of gaseous and particulate residues. **S. Brochu**, I. Poulin, D. Faucher, E. Diaz, M. R. Walsh
209. Gaseous and particulate matter emitted during live firing of artillery guns. **E. Diaz**, I. Poulin
210. Remediation of surface soils contaminated with energetic materials by thermal processes. **I. Poulin**
211. Residues from open burning of gun propellant. **E. Diaz**, I. Poulin, S. Brochu, A. Marois, A. Gagnon
212. Soil vadose zone chemistry of TNT and RDX under water-unsaturated conditions. **C. L. Price**, M. Chappell, A. J. George, G. Bourne, L. Ford, B. E. Porter
213. Reductive perchlorate degradation under water-unsaturated soil conditions.  
**M. Chappell**, A. J. George, B. Porter, C. L. Price
214. Thermal treatment of composition B residues by wildfire and managed burns.  
**R. A. Price**

## Section F

Salt Palace Convention Center  
Hall 5

### Evaluation of the Sustainability of Drinking Water Technologies: Application in the Developed World

Cosponsored by AEESP

A. T. Cooper and A. Lindner, *Organizers*

C. J. Clark, *Organizer, Presiding*

## 6:00–8:00

215. Interpretation of fluorescence spectra for characterization of trihalomethanes precursors in source water: Scatters removal and principle component analysis.  
**K. Punburananon**, T. F. Marhaba
216. Solar photocatalytic disinfection of water in developing countries. **D. D. Dionysiou**, M. Pelaez, E. R. Bandala, L. González, P. Dunlop, J. A. Byrne
217. Application of the principles of negligible depletion to colorimetric-solid phase extraction. **L. M. Siperko**, M. D. Porter, R. J. Lipert

## Section G

Salt Palace Convention Center  
Hall 5

### Frontiers in Water Reuse: Detection, Advanced Treatment and Environmental Fate of Contaminants of Emerging Concern

E. P. Kolodziej and D. M. Cwierny,  
*Organizers, Presiding*

## 6:00–8:00

218. Comparison of extraction and derivatization methods for use in GC/MS analysis of endocrine-disrupting compounds in water.  
**W.-S. Kim**, A. Do, D. H. Yeh, J. A. Cunningham
219. Evaluation of chemically assisted MF and UF systems for PPCP removal.  
**S. Sathyamoorthy**, C. A. Ramsburg
220. Examination of the role of excited state triplet natural organic matter in the photo-degradation of organic contaminants.  
**K. E. Daumit**, D. E. Latch, C. N. Goodwin, J. L. Gray, G. R. Aiken

221. Mechanisms of triazole corrosion protection in cooling systems using secondary treated municipal wastewater as makeup water. **M.-K. Hsieh**, H. Li, S.-H. Chien, D. A. Dzombak, R. Vidic
222. Mineral deposition in cooling systems when secondary municipal wastewater is used: Modeling, kinetics, and inhibition.  
H. Li, R. Vidic, M.-K. Hsieh, D. A. Dzombak
223. Permanganate oxidation of pharmaceutically-active compounds in utility source waters: Kinetic model validation.  
**H. M. Martin**, L. Hu, T. J. Strathmann
224. Potential effect of micropollutant (TCEP) in reclaimed water for reuse purpose.  
**X. Ren**, I. S. Kim, Y. Lee, H. Han
225. Quantifying pCBA radical chemistry: Kinetics of hydroxylated product formation and decay. **S. P. Mezyk**, D. F. R. Doud, F. Rosario-Ortiz, S. A. Snyder
226. Transformation of sulfonamide antibiotics in agricultural soils under varying biogeochemical conditions. **J. L. Mohatt**, K. T. Finneran, T. J. Strathmann

## Section H

Salt Palace Convention Center  
Hall 5

## New Energy Technology

J. Marwan, *Organizer, Presiding*

## 6:00–8:00

227. Low energy nuclear reactions in gas phase experiments: An update.  
**J.-P. Biberian**

## THURSDAY MORNING

## Section A

Hilton  
Alpine Ballroom West

### Environmental Distribution, Degradation, and Mobility of Explosives and Propellant Compounds

M. Chappell, *Organizer, Presiding*

- 8:30 228. Degradation products of TNT after Fenton oxidation. **C. W. Jarand**, K. Chen, R. B. Cole, D.-T. Pham, S. F. Lincoln, M. A. Tar
- 8:50 229. Computational predictions of environmentally important physical properties of explosives. **Y. Kholod**, **L. Gorb**, F. Hill, M. Qasim, J. Leszczynski
- 9:10 230. Transport of RDX and TNT from Composition B explosive during simulated rainfall. **R. A. Price**, M. Bourne, J. Lindsay, J. Cole
- 9:30 231. Fate and effects of TNT and RDX released from Composition B fragments in marine microcosm exposures. **G. Rosen**, G. R. Lotufo, W. Wild
- 9:50 Discussion.
- 10:10 232. Photolysis of 2,4,6-trinitrotoluene in seawater: Effects of salinity and nitrate concentration. **D. W. O'Sullivan**, J. R. Denzel, D. J. Luning Prak
- 10:30 233. Photolysis of TNT examined by multinuclear NMR. **K. Thorn**, L. G. Cox
- 10:50 234. Quantifying natural attenuation of hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) in groundwater using compound specific ( $\delta^{15}\text{N}$  and  $\delta^{18}\text{O}$ ) isotope analysis. **A. Bernstein**, **Z. Ronen**, E. Adar, R. Meckenstock, W. Stiehr

## Section B

Hilton  
Canyon A

### Nanotoxicology: Ecotoxicity of Manufactured Nanomaterials

Cosponsored by NANO

N. F. Savage and S. R. Al-Abed,  
*Organizers*

## 8:30 Introductory Remarks.

- 8:40 235. Aquatic toxicity of carbon-based nanomaterials at sediment-water interfaces. **B. Deng**

- 9:05 236. Bacteria-quantum dot interactions: Toward an environmental perspective.  
**D. M. Aruguete**, J. S. Guest, N. G. Love, M. F. Hochella Jr.
- 9:30 237. Correlations between surface structure and toxicity of nanoparticles.  
**P. K. Dutta**, W. J. Waldman
- 9:55 Intermission.
- 10:10 238. High throughput screening as an enabling technology for studying the ecotoxicology of nanomaterials. **H. A. Godwin**
- 10:35 239. Nanostructured metal oxides: Syntheses, properties, and nanotoxicology.  
**W. H. Suh**, A. M. Horst, J. H. Priester, G. D. Stucky, P. A. Holden
- 11:00 240. Novel sensors for quantitation and cytotoxicity of selected nanomaterials.  
**S. N. Kikandi**, Q. Wang, O. A. Sadik, K. E. Varner

### Geochemical Processes, Reactivity, and Applications of Manganese Oxides

Sponsored by GEOC, Cosponsored by ENVR and INOR

## THURSDAY AFTERNOON

## Section A

Hilton  
Alpine Ballroom West

### Environmental Distribution, Degradation, and Mobility of Explosives and Propellant Compounds

M. Chappell, *Organizer, Presiding*

- 1:30 241. RDX and HMX destruction by sulfides and black carbons. **K. Dana**, W. A. Mitch
- 1:50 242. Fate of nitroaromatic (TNT) and nitramine (RDX and HMX) explosives on mineral surfaces. **T. A. Douglas**, M. Walsh, A. M. Jones, T. P. Trainor, C. J. McGrath, C. A. Weiss
- 2:10 243.  $\text{TiO}_2$  photocatalytic degradation of phenylarsonic acid. **S. Zheng**, Y. Cai, K. E. O'Shea
- 2:30 244. Ecotoxicology of munitions constituents in the marine environment.  
**G. R. Lotufo**, G. Rosen, W. Wild
- 2:50 245. Accumulation of trinitrotoluene (TNT) in aquatic and terrestrial invertebrates: Formation and persistence of unextractable biotransformation products.  
**J. Belden**, C. K. Chambliss, G. R. Lotufo
- 3:10 246. 2,4,6-Trinitrotoluene mineralization and incorporation by natural bacterial assemblages in the coastal ecosystems.  
**M. T. Montgomery**, T. J. Boyd, J. P. Smith, S. E. Walker, C. L. Osburn

## Section B

Hilton  
Canyon A

### Nanotoxicology: Ecotoxicity of Manufactured Nanomaterials

Cosponsored by NANO

N. F. Savage and S. R. Al-Abed,  
*Organizers*

- 1:30 247. Metal-containing nanoparticles: Effects on a beneficial soil pseudomonad.  
**A. J. Anderson**, P. Gajjar, D. W. Britt, W. Huang, W. P. Johnson
- 1:55 248. Quantification of the interaction between manufactured nanomaterials and bacteria using atomic force microscopy.  
**Y. Chen**
- 2:20 249. Stability of CdSe/ZnS quantum dots in freshwater and the acute toxicity to *Daphnia magna*. **H. E. Pace**, J. F. Ranville, B. P. Jackson

### Geochemical Processes, Reactivity, and Applications of Manganese Oxides

Sponsored by GEOC, Cosponsored by ENVR and INOR

‡ Cooperative Cosponsorship