



ON-SITE MEETING PROGRAM



**237th American Chemical Society
National Meeting & Exposition
Salt Lake City, UT
March 22 – 26, 2009**



338. Formation dynamics of secondary phase of poly(9,9-dioctylfluorene) in solution. **C. W. Cone**, D. A. Vandenberg
339. Hydrogen detection by polyaniline nanofibers: Effect of the electrode metal. **J. D. Fowler**, S. Virji, R. B. Kaner, **B. H. Weiller**
340. Hydrogen-deuterium atom exchange in photolyzed methane-water ice mixtures. **A. S. Weber**, P. V. Johnson, R. Hodyss
341. Infrared spectra of $K^+(APE)(H_2O)_n$. **A. L. Nicely**, J. M. Lisy
342. Ion exclusion and acidity of ice films. **K. F. Searles**, R. R. H. Michelsen
343. IR Diode laser study of collision energy transfer between tetrafluorobenzene isomers and CO_2 . **K. Kim**, A. M. Johnson, E. T. Sevy
344. Isothermal titration calorimetry studies of thrombin interaction with tetrapeptides reversible inhibitors. **C. C. Clement**, M. Philipp
345. Kinetic study of hydrolysis of ATP and GTP at 37 °C and a mechanistic study by theoretical calculations. **B. A. Dougan**, H. Liu, Y.-D. Wu, Z.-L. Xue
346. Kinetics study of the reaction of OH with xylenes at 1-9 Torr and 240-340K using the relative rate/discharge flow/mass spectrometry technique. **D. N. Mehta**, A. Nguyen, Z. Li
347. Lanthanide ion reduction by an intense femtosecond laser pulse. **N. Nakashima**, D. Nishida, M. Kusaba, T. Yatsuhashi
348. Laser assisted folding of binary chromophore organic glasses. **B. C. Olbricht**, P. A. Sullivan, J. A. Davies, T. R. Ewy, B. E. Eichinger, B. H. Robinson, P. J. Reid, L. R. Dalton
349. Methane activation by Os^+ . **L. G. Parke**, P. B. Armentrout
350. Morphology-controlled synthesis of lead chalcogenide nanocrystals using vapor transport and solvothermal methods. **S. Y. Jang**, J. Park, J. W. Cho, H. S. Kim, Y. J. Cho, C. H. Kim
351. Novel phenomena of crystallization and crystal growth by photon pressure of a focused cw laser beam. **H. Masuhara**, T. Sugiyama
352. Novel preparation and characterization of doped para-hydrogen solids. **B. B. Smith**, J. S. Winn
353. Phase transitions in Langmuir films of n-perfluorocarboxylic acids. **K. G. Nelson**, C. D. Vecitis, E. M. Spain, N. F. Dalleska
354. Probing molecular structures of silicone elastomer-silane interfaces. **A. V. Vázquez**, N. E. Shephard, S. Rhodes, Z. Chen
355. Raman spectra of 1,3-butadiene- d_0 and - d_6 and their torsional potential energy function. **P. Boopalachandran**, J. Laane, N. C. Craig
356. Reactive and nonreactive interactions of thiophene with WS₂ and MoS₂ fullerene-like nanoparticles. **A. Sand**, J. Goering, U. Burghaus, B. W. Arey, O. Eidelman, A. Zak, R. Rosentsveig, R. Tenne
357. Reduction of poly-2,7-(9,9-dihexylfluorene) molecular wires to form polyanions. **L. Zaikowski**, C. Gelfond, E. D. Selvaggio, S. Asaoka, N. Takeda, A. Yang, J. Miller
358. Refractive index effects on molecular electronic oscillator strengths and radiative decay rates in supercritical fluids. **B. J. Hrnjez**, J. A. Saperia, J. J. Hefter
359. Relaxation of highly vibrationally excited trifluorobenzene by collisions with CO_2 . **A. M. Johnson**, K. Kim, E. T. Sevy
360. Solid-state NMR and quantum chemistry of melamine-cyanuric acid. **G. S. Harbison**, M. Kinde-Carson
361. Solvent effects in extraction of carboxylic acids. **M. Prezhdo**, L. P. Loginova, V. V. Prezhdo
362. Studies of hydrocarbon evaporation. **R. S. Booth**, A. N. VanTilburg, C. Pursell, P. Kelly-Zion
363. Suggestion for rationalization of anomalous dispersion of excitability waves in the ferriin-catalyzed Belousov-Zhabotinsky (BZ) reaction with 1,4-cyclohexanedione as the organic substrate. **R. M. Boger**, **R. J. Field**
364. Synthesis and characterization of silver nanorods and nanotriangles. **A. Roth**, H. McBride, A. M. Brun, I. Gryczynski, T. Shtoyko
365. The gas-phase reaction of atomic chlorine with ethylene: Experiments and computations. **I. M. Alecu**, K. E. Kerr, K. Thompson, N. Wallace, Y. Gao, **P. Marshall**
366. The photocatalytic activity of nanoparticles-carbon nanotube and -TiO₂ hybrid nanostructures toward decomposition of 1,4-dioxane and methylene blue. **D. M. Jang**, J. Park
367. The protonation of 1-pentanol and tert-butanol in sulfuric acid solutions at cold temperatures. **A. V. MacLauchlan**, R. R. H. Michelsen
368. Thermal stability and decomposition kinetics of *N,N*-diethyl-*N'*-(4-chloro)benzoylthiourea and its copper(II) and nickel(II) complexes. **H. Arslan**, G. Binzet, N. Külüçü, U. Florke
369. Time-resolved dynamics of photoelectrons in He droplets: VUV-IR study with femtosecond resolution. **O. A. Kornilov**, C. C. Wang, A. Healy, M. Leonard, S. Peng, S. R. Leone, O. Gessner, D. M. Neumark
370. Toward bulk materials with a negative index of refraction in the visible. **S. Roy**, T. F. Magnera, J. Michl
371. Vibrational spectroscopic studies of host/guest interactions in cyclophane/anthracene complexes. **T. Buthelezi**
372. Water bonding and structure in the presence of ions at the fluoride/water interface. **A. J. Hopkins**, G. L. Richmond
373. Crystallization kinetics of an induced crystallization studied in nanocolloidal octylecyanobiphenyl liquid crystal gels. **D. Sharma**
374. Architectural complexity and charge transfer in metal-organic coordination networks at surfaces. **S. L. Tait**, A. Langner, T.-C. Tseng, N. Lin, K. Kern
375. Factors that determine molecular structure of polystyrene surfaces. **A. D. Curtis**, B. J. Nielson, S. B. Moxley, A. D. Quast, J. E. Patterson
376. Carbon-silica composite mesoporous films: Impact of silica content on conductivity and modulus. **L. Song**, D. Feng, C. G. Campbell, A. M. Forster, D. Zhao, B. D. Vogt
377. Catalytic nanocutting of graphene sheets. **L. Ci**, L. Song, W. Gao, D. Jariwala, P. M. Ajayan, A. Elias
378. Effects of carbon source geometry and reactivity on the CVD growth of single-walled carbon nanotubes. **C. Beasley**, B. M. Clemens, H.-S. P. Wong
379. Fast nonlinear ion transport via field-induced hydrodynamic slip in sub-20nm hydrophilic nanofluidic channels. **U. Vermesh**, J. W. Choi, O. Vermesh, R. Fan, J. Nagarath, J. R. Heath
380. Gold nanorods with tunable size evenly distributed in the channels of mesoporous silica. **Z. Li**, R. M. Richards, C. Kuebel
381. Individually-wired nanoelectrodes for a 3-D nanostructured battery systems. **D. Teeters**, P. L. Johnson
382. UHV-STM investigations on DNA bases. **W. Xu**, R. Otero, M. Lukas, R. Kelly, E. Laegsgaard, L. Kantorovich, F. Besenbacher

Section D

Salt Palace Convention Center
Hall 5

New Developments in Energy Conversion and Light-Harvesting

M. Head-Gordon, *Organizer*

7:30-9:30

383. Chemical mapping of donor/acceptor polymer thin film morphologies: Effect of processing conditions. **Y. Gao**, J. K. Grey
384. Degradation of organic compounds by photocatalytically active MoS_2 and WS_2 particles. **D. James**, T. Zubkov
385. Effect of surface active agents on the photoluminescence of titanium dioxide nanocrystals. **C. C. Rich**, J. L. McHale
386. Long lived charge separation in perylene-quinone dyad using proton coupled electron transfer. **P. Kucheryavy**, G. Li, K. D. Glusac

387. Molecular triads comprised of boron dipyrin-C60 dyad connected to either an dipyrin or electron donating entity to probe sequential energy/electron transfer events. **C. A. Wijesinghe**, F. D'Souza
388. Nanoscale insights into the internal structure of porphyrin nanorods. **B. A. Friesen**, U. Mazur, J. L. McHale, K. Nishida
389. Near-field scanning optical microscopy for high resolution photocurrent and time correlated single photon counting lifetime measurements in organic photovoltaics. **M. S. Glaz**, D. A. Vandenberg
390. Noncovalent aggregates of 1,3-diphenylisobenzofuran for singlet fission studies. **M. B. Smith**, J. C. Johnson, J. Michl
391. On 1-D nanostructure-guided chain reactions: Harmonic interactions. **N. Nair**, M. S. Strano
392. Solvent effects on dye structure and electron transport properties of sensitized nanocrystalline titanium dioxide. **J. A. Downing**, J. L. McHale
393. Spectroscopy of betanin and its application as a sensitizer for TiO_2 based dye-sensitized solar cells. **C. S. Sandquist**, J. L. McHale
394. Charge delocalization and separation in type II tunneling structures of CdTe and CdSe nanocrystals by surface photovoltage spectroscopy. **D. Gross**, I. Mora Seró, T. Ditttrich, A. S. Susha, A. L. Rogach, E. Da Como, J. Feldmann
395. Withdrawn.
396. Excitonic and vibronic coupling in supra-molecular light harvesting porphyrin complexes probed by resonance Raman spectroscopy. **J. L. McHale**, U. Mazur, B. A. Friesen
397. Interfacial structure and dynamics at the electrode/organic interface. **M. L. Blumenfeld**, M. P. Steele, O. L. A. Monti
398. Photoluminescence and Raman spectroscopy of titanium dioxide nanotubes. **C. C. Mercado**, J. L. McHale
399. Rate of glucose equivalent production in C4 plants and the effect of pressure and temperature. **A. Panda**, S. N. Datta
400. The effect of surface ligands on optical and electronic spectra of semiconductor nanoclusters. **S. V. Kilina**, S. A. Ivanov, S. Tretiak
401. Ultrafast exciton dynamics in a DNA duplex helix and its application to nonlinear spectroscopy. **H.-D. Kim**, Y. Tanimura, M. Cho

406. Coarse-grained ions without charges: Improving computational efficiency by eliminating electrostatic interactions. **R. C. DeMille**, V. Molinero
407. Developing polarizable force fields from ab initio calculations: A critical analysis of methods. **J. R. Hammond**, S. S. Xantheas, K. Kowalski
408. Solvation of ions: Molecular dynamics simulation using combined quantum mechanical, effective fragment potential and continuum solvation model. **H. Li**, P. Su

Section F

Salt Palace Convention Center
Hall 5

Convergence between Theory and Experiment in Surface Chemistry and Catalysis

M. Head-Gordon, *Organizer*

7:30-9:30

409. Ab initio study of Au_3 cluster interactions with titanium dioxide. **Y. Kholod**, B. Njegic, M. S. Gordon
410. Catalysis of Henry reaction in mesoporous silica nanospheres. **S. A. Nedd**, M. S. Gordon
411. Chemical structure of CuO-NiO/chabazite oxygen carrier in chemical-looping combustion. **E. M. Eyring**, P.-H. Liao, H. P. Wang
412. CO oxidation and ethylene hydrogenation over one nanometer bimetallic RhPt particles. **W. Huang**, Y. Li, J. N. Kuhn, C.-K. Tsung, G. A. Somorjai
413. Measuring surface interactions using fluorescence correlation spectroscopy. **C. R. Daniels**, C. G. Reznik, C. F. Landes
414. Methanol oxidation on neutral iron oxide clusters in the gas phase. **Y. Xie**, F. Dong, E. R. Bernstein
415. Partitioning behavior of perchlorate vs. chloride ions in aqueous solutions: An electron spectroscopy and first principles MD simulations study. **S. Ghosal**
416. STM Study of adsorption sites of size-selected Au_1 , V_x , and V_xO_y clusters on a $TiO_2(110)-1\times 1$ surface. **X. Tong**, S. P. Price, C. Ridge, L. B. Benz, P. Kemper, H. Metiu, M. T. Bowers, S. Baratto

Section E

Salt Palace Convention Center
Hall 5

Progress in Polarizable Force Fields and Simulation

M. Head-Gordon, *Organizer*

7:30-9:30

402. Applications of a novel QM/MM method incorporating a polarizable force field. **C. F. Williams**
403. Effects of sodium hydroxide on the solvation of dimethyl-succinate in water: A computational study. **X. Sun**, Y. Cao, S. Niwayama, W. L. Hase, L. X. Dang
404. Fluctuating-charge models in bond space and their exact reformulation in atomic space. **J. Chen**, D. Hundertmark, T. J. Martínez
405. Atomistic molecular dynamics simulations of poly (ethylene oxide) aqueous solutions as a function of concentration and temperature using polarizable force field. **O. N. Starovoytov**, O. Borodin, D. Bedrov, G. D. Smith

THURSDAY MORNING

Section A

Salt Palace Convention Center
250 A

Advances in Electronic Structure Theory and First Principles Dynamics Challenging Applications

C. D. Sherrill and G. Galli, *Organizers*B. G. Sumpter, *Presiding*

- 8:30 417. Ab initio molecular dynamics study of the density of liquid water: How reliable are DFT-based simulations of wet systems? **M. Fernandez-Serra**
- 9:10 418. Many-body corrections to density functional theory level alignment at organic-inorganic hybrid interfaces using quantum Monte Carlo calculations. **Y. Kanai**, Z. Wu, J. C. Grossman
- 9:50 419. Melting of iron at Earth's core conditions from quantum Monte Carlo free energy calculations. **D. Aife**
- 10:30 Intermission.
- 10:50 420. Reduced dimensional studies of roaming radicals. **L. B. Harding**, S. J. Klippenstein, Y. Georgievskii
- 11:30 421. Tackling thermal effects on molecular chiroptical properties. **F. Furche**

‡ Cooperative Cosponsorship



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NOTE: Abstracts public availability on January 26, 2009; rooms and times subject to change.

Thermal stability and decomposition kinetics of *N,N*-diethyl-*N'*-(4-chloro)benzoylthiourea and its copper(II) and nickel(II) complexes

PHYS 368

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N,N-diethyl-*N'*-(4-chlorobenzoylthiourea) and its Ni(II) and Cu(II) complexes have been synthesized and characterized by elemental analysis, FT-IR spectroscopy and ¹H-NMR spectroscopy. The thermal decomposition reaction of the compounds was investigated by thermogravimetry (TG) and differential thermal analysis (DTA) techniques. A gas chromatography-mass spectrometry combined system was used to identify the products during pyrolytic decomposition. The end-products of decomposition were identified by TG and X-ray powder diffraction techniques. The kinetic analysis of the thermogravimetric data was performed by using the Ozawa method. Relationship between thermal stability and crystal structure of the ligand was also discussed.

[General Experimental Physical Chemistry](#)

7:30 PM-9:30 PM, Wednesday, March 25, 2009 Salt Palace Convention Center -- Hall 5, Poster

[Division of Physical Chemistry](#)

[The 237th ACS National Meeting, Salt Lake City, UT, March 22-26, 2009](#)