Sunday, July 11, 2011: Welcoming Reception 6:00 p.m. Stata (Building 32) 4th floor, R&D Common

MONDAY MORNING, JULY 11, 2011

8:30 AM Conference Welcome and Overview
Session Chair: Nick Williams
Room 32-123

8:40 AM Plenary Lecture: KINETIC STUDIES OF CHIRAL AMPLIFICATION IN AUTOCATALYTIC REACTION
  Donna Blackmon, Scripps Research Institute

9:00 AM Poster Highlights

9:50 AM Refreshment Break

10:20 AM PROBING KINETICS USING SYNCHROTRON RADIATION [69]
  Musahid Ahmed

11:05 AM ULTRAFAST TIME-RESOLVED X-RAY ABSORPTION SPECTROSCOPY: WATCHING ATOMS DANCE [270]
  Christopher Milne

11:45 AM FREE RADICAL HETEROGENEOUS OXIDATION TRAJECTORIES [114]
  Kevin Wilson
  Lunch Discussion to follow

12:00 PM THE DEVELOPMENT OF QUANTITATIVE INSIGHT INTO ALKENE METATHESIS CHEMISTRY [120]
  Sara Kyne

12:25 PM Break for Lunch (see map and restaurant info)
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Presentations</th>
</tr>
</thead>
</table>
| 1:50 PM  | Rate Calculations Chair: Judit Zador Room 32-123                       | 1:50 PM MULTI-STRUCTURAL VARIATIONAL TRANSITION STATE THEORY [#265] Donald Truhlar  
2:15 PM  | Analysis of the main reaction pathways active during cyclopentadiene pyrolysis [#195] Carlo Cavallotti  
2:40 PM  | 4.00 PM SEMI-CLASSICAL TRANSITION STATE THEORY APPLIED TO MULTIWELL CALCULATIONS ON THE OH+CO2 REACTION [#216] Ralph Weston  
3:05 PM  | Non-Born–Oppenheimer molecular dynamics and transition state theory study of the spin-forbidden H + HO2 → H2O + O(3P) reaction [#177] Ahren Jasper  
3:30 PM  | Thermochemistry, reaction paths and kinetics on the isooctane radical reactions with O2 [#240] Suwarwee Snitsiriwat  
3:55 PM  | Theoretical study of the mechanism and kinetics of the reaction of phenyl radical with propylene [#238] Vadim Kislov  
|          | Rate Estimation Chair: Elke Goos Room 32-141                           | 1:50 PM DETAILED CHEMICAL KINETIC MODELING OF JP-10 (EXOTETRAHYDROCYCLOPENTADIENE) HIGH TEMPERATURE OXIDATION [#51] Gregory Magoon  
2:15 PM  | Reaction intermediates at low temperatures: reaction of nitrogen monoxide with dioxygen in cold glassy hydrocarbons [#159] Willem Kappersmol  
2:40 PM  | Tree structure for intermolecular hydrogen abstraction in hydrocarbons (CH) and generic rate constant rules for abstraction by vinyl radical [#233] Sumathy Raman  
3:05 PM  | Rate constant estimation for large chemical kinetic models and application to biofuels [#178] William Pitz  
3:30 PM  | Reactions CH3 + OH, CH3 + CH3, and OH + OH studied over 1 - 100 bar pressure and 298 - 715 K temperature ranges [#223] Lev Krasnoperov  
3:55 PM  | Compatibility of experimental data from thermal and chemical activation [#168] Wing Tsang  
|          | Low T Chair: Christa Fittschen Room 32-144                              | 1:50 PM MASTER EQUATION CALCULATIONS FOR HYDROCARBON AND NITROGENOUS SPECIES REACTION RATE CONSTANTS AT LOW PRESSURES AND TEMPERATURES [#113] Gregory Smith  
2:15 PM  | Experimental investigations of radical-molecule reactions using low temperature supersonic flows [#254] Ian Sims  
3:05 PM  | Kinetics of NOx removal by peroxodisulfate activated by temperature, transition metals ions and ultrasound [#200] Yusuf Adewusi  
3:30 PM  | Theoretical study on the mechanism and kinetics of the reaction of phenyl radical with propylene [#238] Vadim Kislov  
3:55 PM  | Pulsed Laval nozzle studies of the kinetics of reactions between OH and various oxygenated VOCs at very low temperatures [#141] Wing Tsang  
|          | Catalysis 2 Chair: Guy Marin Room 32-155                                 | 1:50 PM GAS PHASE KINETICS OF 1,3 BUTADIENE OXIDATION TO FURAN AND ISOBUTENE TO METHACROLEIN OVER BISMUTH MOLYBDATE CATALYSTS [#255] Patrick Mills  
2:15 PM  | Oxidation of cis-cyclooctene on heterogeneous Mn-TMTACN catalysts [#224] Kathryn Bjorkman  
2:40 PM  | Kinetics of NOx removal by peroxodisulfate activated by temperature, transition metals ions and ultrasound [#200] Yusuf Adewusi  
3:05 PM  | Kinetic study of cobalt(II) catalyzed hydroperoxide activation [#142] Ive Hermans  
3:30 PM  | Metallo-catalysts for destruction of neutral organophosphorus pesticides in alcohol, large rate accelerations brought on by a medium effect [#18] R. Stan Brown  
4:20 PM  | Adjourn to Poster Session (Sala de Puerto Rico, Building W-20 2nd floor) |
### TUESDAY MORNING, JULY 12, 2011

**Plenary Lecture:** HOMOLYTIC C-H BOND ACTIVATION: THE ROLE OF OXYGEN-CENTERED RADICALS AND MECHANISTIC ASPECTS  
*Helmut Schwarz, Technische Universität Berlin*

**Session Chair:** Iva Hermans  
**Room 32-123**

#### 8:30 AM
- **Plenary Lecture:** HOMOLYTIC C-H BOND ACTIVATION: THE ROLE OF OXYGEN-CENTERED RADICALS AND MECHANISTIC ASPECTS  
  Helmut Schwarz, Technische Universität Berlin

#### 9:30 AM
- Poster Awards from Monday

#### 9:45 AM
- **Refreshment Break**

#### 10:15 AM
- **RATES OF H-ABSTRACTION FROM OXYGENATES; HOW DOES THESE DIFFER FROM HYDROCARBONS?**  
  Henry Curran
- **CHEMICAL ACTIVATION REACTIONS OF CYCLIC ALKANE, ETHER AND TRICYCLO DECANE RING-OPENED DIRADICALS WITH MOLECULAR OXYGEN: THERMOCHEMISTRY, REACTION PATHS AND KINETICS**  
  Ittaso Auzumendi-Murua
- **MODELING THE THERMAL REARRANGEMENTS OF BICYCLIC MONOTERPENES**  
  Nick Vandewiele
- **FIRST PRINCIPLES PREDICTION OF RATE COEFFICIENTS IN FREE-RADICAL POLYMERIZATION: SCOPE AND LIMITATIONS**  
  Michelle Coote
- **COMBUSTION OF THE BUTANOL ISOMERS: REACTION PATHWAYS AT ELEVATED Pressures FROM LOW-TO-HIGH TEMPERATURES**  
  William Green
- **MULTI-SPECIES MEASUREMENTS OF N-BUTANOL PYROLYSIS BEHIND REFLECTED SHOCK WAVES**  
  David Davidson
- **DETAILED KINETIC MODELING OF PYROLYSIS AND COMBUSTION OF N-BUTANOL**  
  Alessio Frassoldati
- **RATES AND MECHANISMS OF THE THERMAL GAS-PHASE ISOMERIZATIONS AND DECOMPOSITIONS OF ETHYLCYCLOPROPANE AND 1,1-DIETHYLCYCLOPROPANE**  
  David Lewis
- **RATE CONSTANTS FOR HYDROGEN-ABSTRACTION BY HO2• FROM n-BUTANOL**  
  Cheng-Wei Zhou
- **Butanol Lunch Discussion to follow**

#### 11:05 AM
- **FIRST PRINCIPLES PREDICTION OF RATE COEFFICIENTS IN FREE-RADICAL POLYMERIZATION: SCOPE AND LIMITATIONS**  
  Michelle Coote
- **REACTIONS OF SULFUR ATOMS WITH H2 AND CS2: THE IMPORTANCE OF SPIN-FORBIDDEN PATHWAYS**  
  Paul Marshall
- **H-TYPE CARRIER-BASED MODELING**  
  Steve Jaffe
- **ACCELERATION OF THE THERMAL DECOMPOSITION OF 1-HEXENE-6-YL RADICALS**  
  Sebastian Peukert
- **MULTI-SPECIES MEASUREMENTS OF N-BUTANOL PYROLYSIS BEHIND REFLECTED SHOCK WAVES**  
  David Davidson
- **C5H6 F**  
  Patrick Lynch
- **HIGH TEMPERATURE RATE CONSTANTS FOR D+C2H6 AND C3H8**  
  Joe Michael
- **HIGH TEMPERATURE DISSOCIATION OF O-BENZYLE AND C6H5F**  
  Patrick Lynch
- **DETAILED KINETIC MODELING OF PYROLYSIS AND COMBUSTION OF N-BUTANOL**  
  Alessio Frassoldati
- **GAS PHASE ION CHEMISTRY: FROM ALPHA NUCLEOPHILES TO ALPHA CENTAURI**  
  Veronica Bierbaum
- **SHOCK TUBE STUDY ON THE REACTIONS NCN + H AND NCN + O**  
  Gernot Friedrichs

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#### 12:45 PM
- **Butanol Lunch Discussion to follow**

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**Afternoon free for Interactions or sightseeing**

**5:00 p.m Poster Session**  Sala de Puerto Rico (Building W-20, Second floor)

**7:00 p.m Conference Barbeque**  Sala de Puerto Rico
## ORAL PRESENTATIONS - Session 4

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<tbody>
<tr>
<td>10:15 AM</td>
<td>INTRODUCTION</td>
<td>Craig Taatjes</td>
<td>32-123</td>
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<tr>
<td>10:25 AM</td>
<td>METHODOLOGY AND INFRASTRUCTURE FOR PREDICTIVE MODELING</td>
<td>Michael Frenklach</td>
<td>32-123</td>
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<tr>
<td>11:05 AM</td>
<td>THE ROLE OF SENSITIVITY ANALYSIS IN MODEL IMPROVEMENT</td>
<td>Alison Tomlin</td>
<td>32-123</td>
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<td>11:45 AM</td>
<td>DETERMINATION OF ARRHENIUS PARAMETERS BASED ON BOTH DIRECT AND INDIRECT MEASUREMENTS</td>
<td>Tamas Turanyi</td>
<td>32-123</td>
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<tr>
<td>10:25 AM</td>
<td>Propyl + O2: DEFINITIVE THEORY ON A PROTOTYPE OF HYDROCARBON OXIDATION</td>
<td>Wesley Allen</td>
<td>32-141</td>
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<tr>
<td>10:40 AM</td>
<td>KINETIC MODEL FOR FLAME SYNTHESIS OF SILICA NANOPIRTELES FROM TEOS</td>
<td>Markus Kraft</td>
<td>32-141</td>
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<tr>
<td>11:05 AM</td>
<td>REACTION RATE RULES FOR HIGH AND LOW TEMPERATURE OXIDATION OF LARGE-2 METHYLALKANES</td>
<td>Mani Sarathy</td>
<td>32-141</td>
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<tr>
<td>11:30 AM</td>
<td>REACTION KINETICS IN INTERSTELLAR CLOUDS OF GAS AND DUST: THE ROLES OF SURFACE AND GAS-PHASE CHEMISTRY</td>
<td>Eric Herbst</td>
<td>32-141</td>
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<tr>
<td>10:15 AM</td>
<td>OBSERVATIONS OF BROMINE EXPLOSIONS IN SMOG CHAMBER EXPERIMENTS ABOVE A MODEL SALT PAN</td>
<td>Cornelius Zetzsch</td>
<td>32-141</td>
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<tr>
<td>10:40 AM</td>
<td>A KINETIC ANALYSIS OF THE SELECTIVE REMOVAL OF ETHYLENE AND PROPYLENE FROM SYNGAS VIA PARTIAL OXIDATION</td>
<td>Stephanie Villano</td>
<td>32-141</td>
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<tr>
<td>11:05 AM</td>
<td>REDUCTION AND ANALYSIS OF DETAILED KINETICS FOR MODELING TiO2 NANOPIRTELES SYNTHESIS IN FLAME REACTORS</td>
<td>Maulak Mehta</td>
<td>32-141</td>
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<tr>
<td>11:30 AM</td>
<td>FORMATION OF FUSED-RING AROMATIC COMPOUNDS FROM THE PYROLYTIC REACTIONS OF THE PHENYL RADICAL WITH ACETYLENE</td>
<td>Andrea Comandini</td>
<td>32-141</td>
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<tr>
<td>10:15 AM</td>
<td>GROUP-ADDITIVE KINETIC MODELING OF BIODIESEL PYROLYSIS: METHYLEDANOATE CASE STUDY</td>
<td>Kevin Van Geem</td>
<td>32-155</td>
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<tr>
<td>10:40 AM</td>
<td>A QUANTITATIVE KINETIC ANALYSIS OF CO ELIMINATION FROM PHENOXY RADICALS</td>
<td>Hans-Heinrich Carstensen</td>
<td>32-155</td>
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### Break for Lunch (see map and restaurant info)
### Wednesday Afternoon, July 13, 2011

#### Oral Presentations - Session 5

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<tr>
<th>Time</th>
<th>Topic</th>
<th>Speaker(s)</th>
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<tr>
<td>1:50 PM</td>
<td>Temperature Dependent Rate Coefficients for OH + Butanol Reactions in the Gas Phase</td>
<td>Max McGillen</td>
</tr>
<tr>
<td>1:50 PM</td>
<td>Application of Pseudo-First-Order Kinetics to Fundamental Organic Reactions</td>
<td>Feng Zhang</td>
</tr>
<tr>
<td>1:50 PM</td>
<td>Direct Dynamics VTST Studies of Unimolecular Reactions of N-Propyl Peroxy Radical</td>
<td>Jedrzej Zador</td>
</tr>
<tr>
<td>1:50 PM</td>
<td>Improved Reaction Mechanism for Combustion of Core Components</td>
<td>Chiral Naik</td>
</tr>
<tr>
<td>2:15 PM</td>
<td>A Thermodynamic and Kinetic Study of the C6H5C•(=O) + O2 Reaction</td>
<td>Joseph Bozzelli</td>
</tr>
<tr>
<td>2:15 PM</td>
<td>Pressure Dependent OH Yields in Alkene + HO2 Reactions: A Theoretical Study</td>
<td>Judit Zador</td>
</tr>
<tr>
<td>2:15 PM</td>
<td>On the Chemical Kinetics of an Unsaturated C7 Ester: Methyl 3 Hexenoate Ignition and Speciation Studies</td>
<td>Scott Wagner</td>
</tr>
<tr>
<td>2:40 PM</td>
<td>Theoretical Study of the Methacrolein – OH Reaction in Air</td>
<td>Gabriel da Silva</td>
</tr>
<tr>
<td>2:40 PM</td>
<td>Development and Application of a ReactFF Reactive Force Field for Hydrocarbon Cracking on a Iron Exchanged Zeolite</td>
<td>Kaushik Joshi</td>
</tr>
<tr>
<td>2:40 PM</td>
<td>Minor Products Analysis during the Low Temperature Oxidation of Alkanes</td>
<td>Frederique Battin-Leclerc</td>
</tr>
<tr>
<td>2:40 PM</td>
<td>An Experimental and Kinetic Modeling Study of N-Propylbenzene Oxidation at Temperatures of 500–1000 K</td>
<td>Saeed Jahanian</td>
</tr>
<tr>
<td>2:40 PM</td>
<td>Improved Reaction Mechanism for Combustion of Core Components</td>
<td>Chiral Naik</td>
</tr>
<tr>
<td>3:05 PM</td>
<td>Isolating Individual Steps in the Oxidation of Large Hydrocarbons: Formation of Secondary Organic Aerosol via the Direct Photolytic Generation of Radical Species</td>
<td>Jesse Kroll</td>
</tr>
<tr>
<td>3:05 PM</td>
<td>Studies of Kinetics and Mechanism of Redox Reaction Between Gold(II) Chloride Complexes and Oxalic Acid</td>
<td>Krysztof Pałkowski</td>
</tr>
<tr>
<td>3:05 PM</td>
<td>Updated Chemical Reaction Mechanism for Methane Combustion at High Pressure</td>
<td>Mayun Goswami</td>
</tr>
<tr>
<td>3:30 PM</td>
<td>Chemical Feedbacks on the Atmospheric Lifetime of NO and NO2 Radicals</td>
<td>Ron Cohen</td>
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<tr>
<td>3:30 PM</td>
<td>Kinetics of COx Formation in MC Oxidation of P-Xylene</td>
<td>Weizhen Sun</td>
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<tr>
<td>3:30 PM</td>
<td>Synchrotron Photoionization Measurements of Biofuel Autoignition Chemistry: Low-Temperature Oxidation of Ketones</td>
<td>Subith Vasu</td>
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<tr>
<td>3:30 PM</td>
<td>Modeling the Combustion of High Molecular Weight Fuels by a Functional Group Approach</td>
<td>Marco Mehl</td>
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<tr>
<td>3:55 PM</td>
<td>First Principle Investigations and Molecular Dynamics Simulations of Heterogeneous Reaction Mechanism of Formaldehyde on Fe(001) Surface and Comparison with Experimental Data</td>
<td>Takahiro Yamada</td>
</tr>
<tr>
<td>3:55 PM</td>
<td>Low-Temperature Peroxy Radical Isomerisations in Alkane Autoxidation and Atmospheric Chemistry</td>
<td>Ivie Hermans</td>
</tr>
<tr>
<td>3:55 PM</td>
<td>Kinetic Results from the Experimental Combustion of Cyclopentadiene Derived from a New CS</td>
<td>Robert Butler</td>
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Adjourn to Poster Session (Sala de Puerto Rico, Building W20 Second Floor)
THURSDAY, JULY 14, 2011

**Plenary Lecture:** A LASER FLASH PHOTOLYSIS STUDY OF CO2 REDUCTION: KINETICS LEADING TO THE DESIGN OF A RENEWABLE REDUCING AGENT - Barry Carpenter, Cardiff University

9:30 AM Poster Awards from Wednesday

9:45 AM Refreshment Break

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<tr>
<td>10:15 AM</td>
<td>KINETICS OF REACTIONS ACCELERATED BY MECHANICAL FORCE [#123]</td>
<td>Stephen Craig</td>
<td>32-123</td>
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<tr>
<td>10:15 AM</td>
<td>KINETICS AND OH YIELD MEASUREMENTS TO CONSTRAIN ENERGY BARRIERS IN THE CH3OCH2 + O2 REACTION [#132]</td>
<td>Paul Seakins</td>
<td></td>
</tr>
<tr>
<td>10:40 AM</td>
<td>ON PIMS STUDY OF METHYLPHENYL OXIDATION: ISOMER-SPECIFIC PRODUCT DETECTION [#244]</td>
<td>Adam Trevitt</td>
<td></td>
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<tr>
<td>10:55 AM</td>
<td>BARRIER COMPRESSION AND TUNNELING IN ENZYME CATALYSED REACTIONS [#21]</td>
<td>Nigel Scrutton</td>
<td></td>
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<tr>
<td>11:05 AM</td>
<td>INTERACTIONS OF THEORY, MODELING AND EXPERIMENT IN DETERMINING THE KINETICS AND MECHANISM OF ELEMENTARY REACTIONS [#242]</td>
<td>Craig Taatjes</td>
<td></td>
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<tr>
<td>11:30 AM</td>
<td>REACTION MECHANISMS OF CARBONATE RADICALS WITH AMINOCARBOXYLATE COMPLEXES IN AQUEOUS SOLUTIONS A PULSE RADIOLYSIS STUDY [#124]</td>
<td>Israel Zilbermann</td>
<td></td>
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<tr>
<td>12:30 PM</td>
<td>IMPROVED RATE CONSTANTS FOR NITROUS ACID DECOMPOSITION IN AQUEOUS SOLUTION AND KINETIC MODELLING OF NOX FORMATION FROM NITROSATING AGENTS [#68]</td>
<td>Mark Rayson</td>
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</table>

**Conference Adjourns**