

**Final Program**  
**7<sup>th</sup> PMUSA Symposium on Fundamental Science**  
**February 28 – March 2, 2006**

<b>Tuesday, February 28, 2006</b>		
7:30	Breakfast	
8:30	Welcome	<i>Peter Lipowicz</i>
8:35	Introduction and Agenda Review	<i>Geoffrey Chan</i>
<b>Session 1: Health Science</b>		
8:40	<b>Plenary Lecture:</b> Cardiovascular Research in the Tobacco Industry – New Concepts and Perspectives?	<i>Martin Unverdorben</i>
9:20	A 12-Month Clinical Evaluation of an Electrically Heated Cigarette Smoking System: Biomarkers of Potential Harm.	<i>B. Zedler, H. Roethig, W. Rees, Q. Liang, R. Kinser</i>
9:40	Studying Differential Gene Expression in Cigarette Smoke-Exposed Model Systems in vitro and in vivo.	<i>S. Gebel, T. Muller</i>
10:05	Cigarette Smoke-Induced Effects on Biological Processes in Rats.	<i>T. Bonk</i>
10:25	Break	
10:45	Molecular Mechanisms of Cellular Defense against Cigarette Smoke-Mediated Oxidative Stress: A Central Role of the Transcription-Factor Nrf2.	<i>A. Hengstermann, C. Knörr-Wittmann, S. Gebel, T. Müller</i>
11:10	A Method to Identify Potentially Bioactive Compounds from Cigarette Smoke.	<i>A. Wittig, T. Hagemeister, R. Stabbert</i>
11:30	Induction of CYP 1A1 Activity by Cigarette Smoke.	<i>C. Euchenhofer</i>
11:50	Lung Inflammation in Rats after Acute Exposure to Cigarette Smoke	<i>P. Vanscheeuwijck, E. Van Miert</i>
12:10	Lunch	
1:10	<b>Plenary Lecture:</b> Potential Contribution of PAHs and Cadmium to Smoking-Related Lung Cancer – a Risk Assessment	<i>Ted Sanders, Anthony Cox</i>

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Tuesday, February 28, 2006		
1:50	Biochemical, immunohistochemical, and molecular biomarkers in rats following inhalation of cigarette mainstream smoke (MS) or a mixture of cigarette sidestream smoke (SS) and MS	<b>D. Weisensee</b> , R. Kindt, E. van Miert, R. Stabbert, P. Kuhl, G. Schepers, S. Gebel, W.K. Schlage, H.-J. Haussmann
2:15	Dilute and Dense Aerosol Transport in the Respiratory Tract	<b>P. Worth Longest</b> , Mohammad Hajaligol
2:35	Kinetic Analysis of Autooxidation of Dihydroxybenzenes Found in TPM of Cigarette Smoke: Relation to Their Cytotoxicity.	<b>Salem Chouchane</b> , Jan B. Wooten, Jennifer Rickets
2:55	The First Model to Predict the Amount of TSNA's Pyrosynthesized during the Smoking Process	Peter Lipowicz, <b>Jeffrey I. Seeman</b> , Roger Walk
3:20	Break	
Session 2: Analytical Methods		
3:40	Investigation on Thermal Behavior of Heavy Metals during Tobacco Pyrolysis by Thermal Vaporization Inductively Coupled Plasma Mass Spectrometry.	<b>Michael J. Chang</b> , John D. Naworal, Catherine M. McNeilly, Chris T. Connell
4:00	EDXRF Quantitative Method Development for Determining the Concentration of Palladium Applied to Tobacco.	<b>Jan Lipscomb</b> , Michael Chang, Tim Danielson, Chris Connell, Stephen Zimmermann
4:20	Development of a Reagentless Optical Sensor for Intracellular Detection of Hydrogen Peroxide Generated from Cigarette Smoke.	Fei Yan, Guy D. Griffin, Sean C. Moffitt, Mark Fisher, Susan E. Plunkett, Kenneth H. Shafer, <b>Tuan Vo-Dinh</b>
4:40	Performance of the Sodim Smoking Puff Analyzer for the Measurement of Human Smoking Topography	<b>Susan Plunkett</b> , Jennifer Smith, Vickie Call, Dawn Anderson, Steve Blankenship, David Self
5:00	Poster Session 1	
6:30	Reception	

Wednesday, March 1, 2006		
7:30	Breakfast	
Session 3: Pyrolysis and Combustion		
8:30	<b>Plenary Lecture:</b> Understanding the Mechanisms of Smoke Formation in a Burning Cigarette.	<b>Mohammad R. Hajaligol</b>
9:10	Does The Benzo[A]Pyrene Found In Mainstream Smoke Arise From The Carbohydrate Fraction Of Tobacco?	<b>Phillip F. Britt, A. C. Buchanan III, J. Todd Skeen, Ralph Ilgner, Juske Horita</b>
9:30	Studies of Solid Phase Biopolymer Pyrolysis.	<b>Robert J. Evans, Heidi M Pilath, Luc Moens, Mark R. Nimlos</b>
9:50	Charring and Pyrolysis of Tobacco or its Components Using a Micro-Pellet Reactor.	<b>Andrew M. Herring, J. Thomas McKinnon</b>
10:10	The Formation of Nitro Polycyclic Aromatic Hydrocarbons during Tobacco Pyrolysis.	<b>A. John Dane, Kent J. Voorhees, Christy Abbas-Hawks, Crystal D. Havey</b>
10:30	Break	
10:50	Investigation of Nitrogen Functional Group Transformation During Tobacco Pyrolysis	<b>R. J. Pugmire, M. S. Solum, Z. Ma, K. Whitty</b>
11:10	Morphological Characterization of Pyrolyzed Avicel Cellulose Treated With Metal Acetates.	<b>Vicki Baliga, Mike Thurston, Thomas McGrath</b>
11:30	A New Perspective on Free Radicals in Cigarette Smoke.	<b>Barry Dellinger, Julien Adunkpe, Lavri Khachatryan, Sophia Masko</b>
11: 50	Investigation of Carbon-Centered Radicals in Cigarette Smoke by Chromatographic and Mass Spectrometric Means.	<b>Judit Bartalis, Jan B. Wooten, W. Geoffrey Chan</b>
12:10	Pyrolysis of Catechol in the Presence of Certain Solids and Gases.	<b>M. J. Wornat, X. Zhang, J. A. Robles, S. Thomas</b>
12:30	Lunch	
Session 4: Nitric Oxide and TSNA		
1:30	Preparation and Characterization of a Selective Nitric Oxide Adsorbents.	<b>W. J. DeSisto, N. Hill, R. Cashon, J. B. Paine III, J. A. Fournier</b>

Wednesday, March 1, 2006		
1:50	NO and Mainstream Smoke: The Mystery of the Missing Molecule	<i>W. David Thweatt, Jon Regrut, Randall Baren, Stephen L. Garrison, Yi-Lei Zhao, Carlos Gonzalez, Manuel Marquez</i>
2:10	Theoretical Studies on Radical Mechanisms for the N-Nitrosation by Nitrogen Oxides in Smoke.	<i>Yi-Lei Zhao, Stephen L. Garrison, W. David Thweatt, Carlos Gonzalez, Manuel Marquez</i>
2:30	Residue Formations of Phosphorous Hydride Polymers and Phosphorous Oxy-Acids during Phosphine Gas Fumigations of Stored Products.	<i>Jason W. Flora, Daryl L. Faustini, Loran E. Byer, Susan E. Plunkett, W. David Thweatt</i>
2:50	Theoretical Exploration of Mechanisms for the Formation of a Yellow 'Polymer' Residue during Phosphine Fumigation.	<i>Stephen L. Garrison, Yi-Lei Zhao, Jason W. Flora, W. David Thweatt, Carlos Gonzalez, Manuel Marquez</i>
3:10	Break	
Session 5: Flavor Encapsulation and Smoke Chemistry		
3:30	Thermodynamics of Concentrated Microgel Suspensions	<i>A. Fernandez-Nieves, L. Rodriguez-Maldonado, I. Suarez, J. J. Lietor-Santos, M. Marquez</i>
3:50	SCF-Assisted Impregnation of Cellulose Acetate Fibers	<i>Shawn Warriner, Michael Clay, Yongchul Kim, Mark A. McHugh, Joseph L. Banyasz, Munmaya K. Mishra</i>
4:10	Some Effects of Filler Glycerin on Cigarette Performance.	<i>R.W. Dwyer, S. Tafur, R.M. Olegario, D.L. Rockwell, M.F. White</i>
4:30	Poster Session 2	
6:00	Banquet	

Thursday, March 2, 2006		
7:30	Breakfast	
Session 6: Emerging Technologies		
8:30	Intrinsic Magnetism in Gold Nano-clusters from Density Functional Theory	<b>Rudolph Magyar</b> , Yamil Simón-Manso, V. Mujica, Manuel Marquez, Carlos Gonzalez
8:50	Rational in Silico Design of Sensors and Catalysts	J. Fredrik Haeffner, <b>Carlos Gonzalez</b> , Manuel Marquez
9:10	Bioactive scaffolds for optimizing engineered tissue formation	<b>Solitaire Lindsay</b> , Steve Massia, Antonio Garcia, Manuel Marquez
9:30	Microencapsulation using Microfluidic Device	<b>Dawei Luo</b> , Zhengdong Cheng, Manuel Marquez
9:50	Darwin on a Chip	<b>Jeremy Agresti</b> , Keunho Ahn, Peter Boul, Manuel Marquez, David A. Weitz
10:10	Synthesis and Self-Assembly of Nearly Monodisperse Nanoparticles of a Naturally Occurring Polymer.	<b>Tong Cai</b> , Zhibing Hu, Manuel Marquez
10:30	Break	
Session 7: Catalysis		
10:50	Photo-Induced Decomposition of Palladium Acetate for Palladium Nanocatalyst Production.	<b>Christopher E. Allmond</b> , Aaron T. Sellinger, James M. Fitz-Gerald
11:10	Nanoparticle Catalysts in Porous Materials	Victor Abdelsayed, Asit Panda, <b>M. Samy El-Shall</b> , Sarojini Deevi
11:30	Supported Transition Metal Oxide Catalysts For Reducing The Amounts Of CO And NO At Low Temperature	<b>Padmanabha Reddy Ettireddy</b> , Sarojini Deevi
11:50	Gold Coated Iron and Iron Oxide Nanostructures: Electronic Structure, Magnetism and Relevance to Biomedical Applications	<b>Q. Sun</b> , M. Marquez, M. Hajaligol, Y. Kawazoe, Q. Wang, P. Jena
12:10	Theoretical Investigation of CO Oxidation on Fe2O3 (100) and (0001) Surfaces	<b>Anil K. Kandalam</b> , P. Jena, S. N. Khanna, B. K. Rao, B. V. Reddy
12:30	Concluding Remarks	<b>Geoffrey Chan</b>
12:35	Lunch	
Meeting Adjourn		

Tuesday, February 28, 2006

Poster Session 1

1-1	A 12-Month Clinical Exposure Evaluation of an Electrically Heated Cigarette Smoking System: Biomarkers of Exposure.	<b>W. Rees, H. Roethig, B. Zedler, Q. Liang, R. Kinser.</b>
1-2	A 12-Month Clinical Evaluation of an Electrically Heated Cigarette Smoking System: Biomarkers of Potential Harm	<b>B. Zedler, H. Roethig, W. Rees, Q. Liang, R. Kinser.</b>
1-3	Blood Pressure Monitoring in Adult Smokers Comparing a Conventional Cigarette to an Electrically Heated Cigarette Smoking System and No-Smoking	<b>M. Unverdorben, A. van der Bijl, M.A.Potgieter, Q.Liang, D.Sica, H.Roethig</b>
1-4	Spiroergometry in Adult Smokers Comparing a Conventional Cigarette to an Electrically Heated Cigarette Smoking System	<b>M. Unverdorben, A. van der Bijl, L.Potgieter, Q.Liang, H.Roethig</b>
1-5	Clinical Exposure Evaluation of a New Electrically Heated Smoking System.	<b>J. Oey, R.D. Kinser, S. Feng, B.L. Nelson, Q. Liang, H.J. Roethig.</b>
1-6	Application of the <i>hmx1</i> Promoter/Enhancer Assay for Routine Determination of Cellular Stress Induced by Cigarette Smoke.	<b>C. Knörr-Wittmann, S. Gebel, T. Müller</b>
1-7	Mutagenicity of the Gas/Vapor Phase of Cigarette Mainstream Smoke from the Reference Cigarette 2R4F.	<b>S. Weber, F.J. Tewes, T.J. Meisgen, J. Diekmann, A. Wittig, D.J. Veltel, K. Rustemeier</b>
1-8	Initial Data on the Effects of Long-Term Cigarette Mainstream Smoke Exposure and High Fat Diet in Apolipoprotein E-Deficient Mice	<b>Lebrun, S, Stinn, W, Weiler, H, Kuhl, P, Friedrichs, B, Urban, H-J, von Holt, K, Wallerath, T, Schleef, R</b>
1-9	Local Deposition of Inhaled Particles by Impaction and Diffusion in an Oral Airway Model	<b>Jinxiang Xi, P. Worth Longest</b>
1-10	Thermophysical Properties of Tobacco and Related Materials.	<b>Bruce E. Waymack, Joseph L. Banyasz</b>
1-11	Constituent Prediction Relationships for Bright Tobacco Grades Based on Multivariate Analysis of <sup>13</sup> C CPMAS NMR Spectra.	<b>Jan B. Wooten</b>
1-12	Application of Infrared Spectroscopy to Evaluate Gas Adsorption Characteristics of Activated Carbon Beads	<b>Jim Lyons-Hart, Milton Parrish</b>

Tuesday, February 28, 2006		
1-13	Evaluation of Activated Carbons Using Inverse Gas Chromatography (IGC) and Nitrogen Porosimetry	<i>Jon Regrut, Milton Parrish, Tim Danielson, Jay Fournier</i>
1-14	The Effect of Paper Permeability on the Cigarette Coal Surface Temperature.	<i>Peishi Chen, Tim Sherwood</i>
1-15	A Modeling Investigation of the Air Flow in a Burning Cigarette.	<i>A. Mhaisekar, M.S. Saidi, M.R. Hajaligol</i>
1-16	A Numerical Investigation of the Intra-Puff Smoke Aerosol Delivery.	<i>M. S. Saidi, M. R. Hajaligol, P. Lipowicz</i>
Wednesday, March 1, 2006		
Poster Session 2		
2-1	Evolution of aromatic ring ensembles from tobacco and tobacco components as detected by NMR	<i>Andrew M. Herring, Steven F. Dec</i>
2-2	Collisionally Induced Dissociation for MBMS Studies	<i>Heidi M. Pilath, Luc Moens, Robert J. Evans, Mark R. Nimlos</i>
2-3	Oxidative Reactivity of Tobacco Char and Formation of Oxides of Carbon and Nitrogen.	<i>X. Chen, P. Li, H. Im, M.R. Hajaligol</i>
2-4	Potential Reactants for Reducing Levels of TSNA.	<i>Rebecca M. Gray, Bruce E. Waymack</i>
2-5	TSNA Formation Mechanisms during Smoking of Burley Tobacco.	<i>Bruce E. Waymack, Rebecca M. Gray</i>
2-6	Adsorptive-Catalytic Nitric Oxide Removal on Activated Carbons at Low Temperature.	<i>Andriy Bahryeyev, Weijun Zhang, Firooz Rasouli.</i>
2-7	Evaluation of Smoke Chemistry for Model Cigarettes Prepared with Tobacco Grown Using Different Fertilizer Application Rates	<i>Randall Baren, Milton Parrish, Charles Harward</i>
2-8	Polyaromatic Resins as Adsorption Materials in Cigarette Filters	<i>Lixin L. Xue, Chares E. Thomas, Harrison L. Yu, Kent B. Koller</i>
2-9	A Fundamental Study into the Flavor Release Mechanism of Micro-Crystalline Cellulose Beads (MCC).	<i>Jon Regrut, Joe Banyasz, George Karles, Jay Fournier</i>
2-10	Flavor Encapsulation and Controlled Release Using Electrospinning and Electrospray.	<i>T. E. McGrath, N. K. Meruva, T. Brown, W. G. Chan</i>
2-11	Highly Nanoporous Fibers by Electrospinning into a Cryogenic Liquid.	<i>Zhihao Shen, Mark McHugh, Raffet Velard, Gustavo Larsen, Manuel Marquez, Jay Fournier, Joseph Banyasz</i>

<b>Wednesday, March 1, 2006</b>		
<b>2-12</b>	Decomposition Chemistry of Poly (Menthyl Acrylate).	<b>Shengsheng Liu</b> , Diane S. Kellogg, Munmaya K. Mishra
<b>2-13</b>	Control of Synthesis Parameters for the Preparation of Active CO Oxidation Catalysts.	Unnikrishnan R Pillai, <b>Sarojini Deevi</b>
<b>2-14</b>	Theoretical Investigation of NO – Carbon surface chemistry	Bappa Chatterjee, <b>B. V. Reddy</b> , Firooz Rasouli
<b>2-15</b>	Liquid Crystalline Phases of Homogeneous Disk-like Particles.	<b>Guangnan Meng</b> , Susanna Wong, Manuel Marquez, Zhengdong Cheng
<b>2-16</b>	Magnetism Induced by Self-Assembled Monolayers on Gold Surfaces: Experimental and Theoretical Evidences.	<b>Yamil Simón-Mans</b> , Rudolph Magyar, Manuel Marquez, Carlos Gonzalez