

Schedule for NECZA, December 10, 2004

8³⁰-9²⁰ **Registration, posters**

9²⁰-9³⁰ **Introduction and account of the 14th IZA Conference, Cape Town**
David Olson, Istvan Halasz

9³⁰-9⁴⁰ **Remembering George Kokotailo**
Günter Kühn & Mike Bennett

9⁴⁰-10³⁰ **The Need of Only Weakly Acidic Catalytic Sites in the Synthesis of Fine and Intermediate Chemicals**
Wolfgang F. Hölderich, Aachen, Germany

10³⁰-11⁰⁰ **Break, posters**

11⁰⁰-11³⁰ **Small Pore Zeolites For Propene/Propane Separation**
David Olson^{a,b}, Miguel Cambor^c and Xiaobo Yang^{b,d}

- a) Rutgers University, New Brunswick, NJ
- b) The University of Pennsylvania, Philadelphia, PA
- c) Institute of Materials Science of Madrid (CSIC), Madrid, Spain
- d) University of Hannover, Hannover, Germany.

11³⁰-12⁰⁰ **In situ XRD, NEXAF and IR study of Binding of NO₂ to Barium Zeolite Y**
Jonathan Hanson, Xianqin Wang, José Rodriguez, Brookhaven National Lab., Upton, NY
Ja Hun Kwak, János Szanyi, Pacific Northwest National Lab., Richland, OR

12⁰⁰-13¹⁵ **Lunch**

13¹⁵-13²⁵ **We congratulate Edith Flanigen to her Lemelson-MIT Lifetime Achievement Award and election into the NATIONAL INVENTORS HALL OF FAME, 2004**
Bonnie Marcus

13²⁵-13⁴⁰ **Formation and Structure of Self-Assembled Silica Nanoparticles in Basic Solutions of Organic and Inorganic Cations**
Joseph Fedeyko, The University of Delaware, Newark, DE

13⁴⁰-14¹⁰ **Catalyst Design and HTE, Perfect Together**
Ivy D. Johnson, Michael C. Kerby, Jeffrey S. Beck, Thomas F. Degnan, and David O. Marler, ExxonMobil Research and Engineering, Annendale, NJ

14¹⁰-14³⁰ **Break**

14³⁰-15¹⁵ **Survey of Nanotube Research**
David E. Luzzi, The University of Pennsylvania, Philadelphia, PA

15¹⁵-15⁴⁵ **Zeolite Co-Stabilizers Use in PVC Applications**
Roman Wypart and Bonnie Marcus, PQ Corporation, Conshohocken, PA

15⁴⁵-16¹⁵ **Structural Modeling of Amorphous Carbons**
Amit Kumar, Norman Wagner, and Raúl F. Lobo, The University of Delaware, Newark, DE

ORAL PRESENTATIONS

The Need of Only Weakly Acidic Catalytic Sites in the Synthesis of Fine and Intermediate Chemicals

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In our days, catalysis research and industrial catalyst development as well as the realization of new process technology are strongly related to environmental compatibility. Thereby solid acid, solid base as well as solid acid-base, bifunctional catalysts play an important role (K. Tanabe and W.F. Hölderich, Appl. Catal. A: General 181 (1999) 399). More than 130 industrial processes are reported to be catalysed by such solids. The use of solid acid catalysts instead of homogeneous Brønsted acids such as H₂SO₄ and Lewis acids such as AlCl₃ avoids the disadvantages of homogeneous catalysis such as high salt formation, corrosion problems, waste disposal, water pollution and problems in sludge treatment. Furthermore, those heterogeneous catalysts can be easily separated from the reaction mixture and can be regenerated if necessary i.e. recyclization and reusability will be given. More than 40% of the catalysts used in industrial processes are based on zeolitic materials.

In the present paper I will demonstrate that only weakly acidic sites in zeolitic catalysts are required in the selective organic synthesis of molecules having functional groups in particular when C-C – bonds have not to be cleaved. Three examples will be presented in whose commercialisation I have been strongly involved. After changing the research interest in the use of zeolites as catalysts from petro chemistry to the synthesis of fine and intermediate chemicals, around 1982, it was recognized already soon that there is a need of gentle acidity in that field. In the production of phenyl acetone by isomerisation of 2-phenyl propanal the Al zeolites are too acidic and cause side product formation. Thus, a somewhat weaker acid catalyst, the Fe ZSM5, had to be applied to achieve 98% selectivity at complete conversion. In the production of tert.-butylamine by direct amination of iso-butene an even more gentle acidity was required to achieve 99,9 % selectivity at acceptable conversion. And finally, in the new caprolactam - process recently commercialised by Sumitomo only extremely weakly acidic silanol nest and vicinal silanol groups of a zeolitic carrier with pentasil structure is needed to run this reaction successfully with 98 % selectivity at 100% conversion.



Small Pore Zeolites For Propene/Propane Separation

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Recently, several 8-ring zeolites have shown potential for the separation of propene from propene/propane mixtures. While all 8-ring zeolites are potential candidates, relatively few have the specific properties required for this separation process. The prospective zeolites include AIPO-14, AIPO-18, ITQ-3, ITQ-12 and pure silica chabazite. Most function on the basis of diffusivity differences. Two show permanent or reversible propane exclusion. The properties of these zeolites and specific potential applications will be discussed.



In situ XRD, NEXAF, and IR Studies of the Binding of NO₂ to Barium Zeolite Y

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The destruction of NO_x species formed during the combustion of fuels is a very important operation for controlling environmental pollution. Using a combination of BaY zeolites and non-thermal plasma promises to ensure its success [1]. Passing the exhaust from combustion over the plasma generates NO₂, following which BaY catalyzes the selective reduction of NO₂ using partially oxidized hydrocarbons also produced in the plasma. *In situ* IR measurements of BaY determined the proportions of NO₃⁻, NO₂⁻, and NO⁺ that bind to the zeolite at different temperatures and after different pre-treatments [2]. Recent NEXAFS measurements at NSLS beam line U7A confirmed the conditions under which these species are observed. We carried out time-resolved XRD measurements at NSLS beam line X7B *in situ* during dehydration, and identified the binding sites of the NO_x species when NO₂ was dosed or removed from the zeolite [3]. In addition, we observed the migration of barium cations within the zeolite and directly correlated this with the amount of bound NO_x. Similar cation migration was observed for fluorocarbon binding to NaY[4]. These studies highlight the value of using multiple *in situ* techniques to understand these complex processes.

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1. Kwak, J.H.; Szanyi, J.; Peden, C.H.F. *J. Catal.* **2003** 220 291.
2. Szanyi, J.; Kwak, J.H.; Peden, C.H.F. *J. Phys. Chem. B* **2004** 108, 3746.
3. Wang, X.; Hanson, J.C.; Szanyi, J.; Rodriguez, J. A. *J Phys. Chem. B.* **2004** 108, 16613.
4. Grey, C.P.; Poshni, F.I.; Gualtieri, A. F., Norby, P.; Hanson, J.C.; Corbin, D.R. *J. Am. Chem. Soc.* **1997**, 119, 1981.



Formation and Structure of Self-Assembled Silica Nanoparticles in Basic Solutions of Organic and Inorganic Cations

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The behavior of silica in the presence of water and structure directing cations is crucial in the development of novel silica materials ranging from porous zeolites and mesoporous materials to Stöber particles. We have completed a room temperature study of the behavior of silica solutions in the presence of both symmetric tetraalkylammonium cations and inorganic cations applying the experimental techniques used in studying colloidal systems (conductivity and pH measurements, and small-angle x-ray and neutron scattering(SAXS and SANS)). For all cations, the low concentration solutions exhibit the same behavior, with nanoparticles forming at a well-defined critical aggregation concentration (CAC). We have discovered that the CAC of these systems is directly related to the pH of the solution, and from this observation, we have applied phase equilibrium principles to explain the interdependence of the formation of nanoparticles and hydroxyl concentration. We have also analyzed the microstructure of these solutions focusing on the morphology and internal structure of the nanoparticles as well as the dependence of nanoparticle structure on the experimental conditions (pH and cation type). These observations will be discussed within the context of zeolite synthesis.



Catalyst Design and HTE, Perfect Together

*Ivy D. Johnson, Michael C. Kerby, Jeffrey S. Beck, Thomas F. Degnan, and
David O. Marler
ExxonMobil Research and Engineering*

The petroleum industry is a diverse industry with a range of products from fuels, to lubes, to chemicals. It is capital intensive with a tremendous drive to use existing hardware through use of advanced catalyst systems. New processes and catalyst systems are required to meet tighter specifications demanded in today's petroleum products. There is a vast array of catalysts used in the petrochemical industry and their discovery, development, and evaluation is not trivial. Until recently, catalyst work could have been viewed as an art form. In an attempt to accelerate the pace as well as demystify catalyst invention and deployment, high throughput experimentation (HTE) design for catalyst synthesis and evaluation is being implemented throughout industry and academia. At ExxonMobil, we are employing "High Throughput Experimentation R&D" - a combination of combinatorial chemistry and HTE to reflect the applicability across all aspects of the development pipeline.

The ExxonMobil and Symyx Technologies five year, alliance is focused on HTE- R&D for the petrochemical industry. This alliance represents the largest commitment to date between an integrated energy/petrochemical company to apply HTE broadly across the Downstream and Chemicals R&D. It brings new tools and techniques into ExxonMobil to discover new materials, evaluate process improvements, and create and apply process models. The topic of this paper will be an overview of ExxonMobil catalyst design and objectives of our HTE R&D program.



Survey of Nanotube Research, Title & abstract to be announced

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Zeolite Co-Stabilizers Use in PVC Applications

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Zeolites are known to be effective co-stabilizers for PVC formulations. In this presentation, the authors discuss Advera® zeolite co-stabilizers produced by the PQ Corporation, their properties and their use in PVC applications. Specifically, the performance of commercial Advera® 401PS and improved Advera® 401F zeolite 4A co-stabilizers was studied in flexible and rigid PVC applications. In case of rigid PVC applications, it was found that, depending on the ingredients content of the PVC formulations, 15 to 50% of the tin mercaptide stabilizer could be replaced by the Advera zeolite co-stabilizer. The PVC formulations with the Advera zeolite had the same or better thermal stability performance. Since Advera co-stabilizers are substantially less expensive than tin stabilizers that they can replace, a significant costs savings can be realized.



Structural Modeling of Amorphous Carbons

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Nanoporous carbons (NPCs) are important materials in industry and are used extensively in applications ranging from gas separation to catalyst support. For gas separations, NPCs display remarkable selectivity for several gases, most noticeably for nitrogen (N₂) and oxygen (O₂). Despite their widespread use, the mechanism of gas transport through these materials is not understood. An understanding of the fundamental mechanism of transport through these materials can help tailor their properties more efficiently and aid in the rational design of membranes. Our goal is to provide a molecular level understanding of configurational diffusion of small molecules through NPCs using computer simulations and experiments.

To address this problem, first we need to develop model NPC structures that are close in physical and chemical properties to the actual carbon samples used in the separations. We have succeeded in developing an algorithm that generates periodic but otherwise 'amorphous' carbons with pre-defined carbon density. We use Monte Carlo (MC) simulations generate the carbon structures. Our new method uses the pyrolysis of polyfurfuryl alcohols as a guideline for generating the carbon structures. The structures generated by our method are composed entirely of sp² carbons. Hydrogen is then added to satisfy the coordination requirements of the carbon atoms. Energy minimization is subsequently carried out on the structures to remove any non-bonded overlaps that might have been created due to the addition of hydrogen. To characterize the carbon structures that we get, we use the pair distribution function (PDF) of the structure, the composition (i.e., the fraction of carbon atoms having three carbon atom neighbors) and the fraction of 5-, 6- and 7-membered rings in the structure. These properties have been found to compare favorably with the values reported for real NPCs in literature. A comparison is made between the PDF of one of our carbon models and the PDF of an actual NPC (density = 1.72 g/cm³, prepared at 800 °C) shows a good correspondence.

POSTER PRESENTATIONS

From Templates to Anionic Bridges: Novel Approaches to Metal-Organic Framework Syntheses

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Zeolites and zeolite-like materials often utilize templates as a structure-directing agents and/or charge balance entities. Within metal-organic frameworks, however, the use of such templates has been absent from synthetic methods. Through hydrothermal synthesis, successful inclusion of 4,4'-dipyridyl and 1,2-bis(4-pyridyl)ethane into several lanthanide and calcium systems has been achieved. Further, a novel form of connectivity within a Sr-adipate system has been discovered, where the anionic salt (nitrate) is seen to bridge two-dimensional Sr-adipate chains into a three-dimensional framework. This demonstrates that the metal salt used in MOF syntheses may, in certain circumstances, influence overall structure topology. Several new structures have thus been synthesized: GWMOF-6 ($[\text{Ln}_2(\text{C}_6\text{H}_8\text{O}_4)_3(\text{H}_2\text{O})_2] \cdot (\text{C}_{10}\text{H}_8\text{N}_2)$) ($\text{Ln} = \text{Pr}^{3+}$, Nd^{3+} , Ce^{3+} , Sm^{3+} , Eu^{3+} , $\text{Eu}^{3+}/\text{Tb}^{3+}$ (50/50)), GWMOF-7 ($[\text{Ca}(\text{C}_6\text{H}_8\text{O}_4)(\text{H}_2\text{O})_2] \cdot (\text{C}_{10}\text{H}_8\text{N}_2)$), GWMOF-8 ($[\text{Ca}(\text{C}_6\text{H}_8\text{O}_4)(\text{H}_2\text{O})_2] \cdot (\text{C}_{12}\text{H}_{12}\text{N}_2)$), and GWMOF-9 ($[\text{Sr}_2(\text{C}_6\text{H}_8\text{O}_4)_2(\text{NO}_3)] \cdot (\text{H}_2\text{O})_4$). Synthesis, structure characterization, and luminescent properties will be presented.



Synthesis, Structural Systematics and Fluorescent Properties of Novel U-M-H₃pdc Coordination Polymers (M = Ag, Cu, Fe; H₃pdc = 3,5-pyrazoledicarboxylic acid)

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Self-assembly under hydrothermal conditions has been employed to synthesize several novel coordination polymeric materials in the U-M-H₃pdc system. Syntheses involving 3,5-pyrazoledicarboxylic acid (H₃pdc) and $\text{UO}_2(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ along with $\text{Cu}(\text{NO}_3)_2 \cdot 2.5\text{H}_2\text{O}$, $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ or AgNO_3 have resulted in the formation of four novel compounds. The structures were determined using single crystal x-ray diffraction. Compound **1** ($\text{UO}_2(\text{C}_5\text{H}_2\text{N}_2\text{O}_4)(\text{H}_2\text{O})$, monoclinic, $P2_1/c$, $a = 6.9556(6)$, $b = 11.302(1)$, $c = 10.5288(9)$, $\beta = 90.057(2)$ and $Z = 4$) consists of a two-dimensional sheet containing the familiar uranyl hexagonal bipyramid. Compound **2** ($\text{Fe}_2(\text{C}_5\text{H}_2\text{N}_2\text{O}_4)_2(\text{OH})_2(\text{H}_2\text{O})_2$, triclinic, $P-1$, $a = 6.688(6)$, $b = 6.942(5)$, $c = 8.617(8)$, $\alpha = 94.38(2)$, $\beta = 101.279(16)$, $\gamma = 108.48(3)$ and $Z = 1$) consists of one-dimensional chains. Compound **3** ($(\text{UO}_2)\text{Cu}(\text{C}_5\text{H}_2\text{N}_2\text{O}_4)_2(\text{H}_2\text{O})_2$, triclinic, $P-1$, $a = 5.1014(7)$, $b = 7.6067(11)$, $c = 10.2910(15)$, $\alpha = 72.380(3)$, $\beta = 86.796(3)$, $\gamma = 84.447(3)$ and $Z = 1$) consists of two-dimensional sheets. Compound **4** ($\text{Ag}(\text{C}_5\text{H}_4\text{N}_2\text{O}_4)_2$, triclinic, $P-1$, $a = 6.8306(2)$, $b = 7.0584(2)$, $c = 13.5569(4)$, $\alpha = 101.6100(12)$, $\beta = 93.4636(12)$, $\gamma = 95.6005(14)$ and $Z = 2$) consists of a molecular structure. Presented will be the synthesis, crystal structures and structural systematics of these novel materials, as well as the fluorescence properties of the uranium-containing compounds.



Template Mediated Synthesis of U-Mo Mineral and High Temperature Phases

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Experimentation using organic templates to direct the formation of uranyl molybdate compounds has led to the synthesis of $C_3H_4N_2[(UO_2)_2(MoO_4)_3]$ (**1**) and $C_2H_3N_3[UO_2Mo_2O_7]$ (**2**). (**1**) was synthesized hydrothermally by reacting $UO_2(NO_3)_2 \cdot 6H_2O$, MoO_3 , and imidazole in a Parr bomb at $180^\circ C$ for 5 days. The product consists of both (**1**) and the mineral iriginite. Changes in the time and temperature of the reaction lead to the formation of only (**1**). The crystal structure of (**1**) is layered and is composed of $[(UO_2)_2(MoO_4)_3]$ sheets containing point shared uranyl pentagonal bipyramids and MoO_4 tetrahedra charged balanced by interlayer imidazolium ions. (**2**) was synthesized hydrothermally by reacting $UO_2(NO_3)_2 \cdot 6H_2O$, MoO_3 , and triazole in a Parr bomb at $180^\circ C$ for 5 days, and only the pure product results. The crystal structure of (**2**) is layered and consists of uranyl molybdate sheets analogous to those seen in the mineral iriginite, with bound triazole molecules replacing some of the coordinated interlayer water molecules. Structural details of (**1**) and (**2**) as well as speculation on the role of iriginite in the two systems will be presented.



The Influence of 4,4'-Dipyridyl on the Topology of U-Carboxylate Systems

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There is interest in uranium chemistry for several reasons including the predictable crystal chemistry of the UO_2^{2+} moiety. UO_2^{2+} is a linear triatomic molecule consisting of a central uranium atom that is triply bonded to two oxygen atoms. This arrangement allows for coordination of ligands orthogonal to the terminal oxygen groups in the UO_2^{2+} ion, and hence the formation of square, pentagonal and hexagonal bipyramidal geometries. The coordination of the UO_2^{2+} ion with flexible difunctional carboxylic acids has been well established, both in the literature and by our group, yet the introduction of an additional rigid ligand to these systems has not been explored. Using this methodology, a new family of structures was synthesized by reacting uranium with flexible aliphatic acids and a rigid ligand (4,4'-dipyridyl) under hydrothermal conditions: **1** ($UO_2(C_6H_8O_4)(C_{10}H_8N_2)$); **2** ($(UO_2)_2(C_5H_6O_4)_3 \cdot (C_{10}H_{10}N_2)(H_2O)_2$) and **3** ($(UO_2)_2(C_7H_{10}O_4)_2(C_7H_{11}O_4)_2 \cdot (C_{10}H_8N_2)(C_{10}H_{10}N_2)(H_2O)_2$). In each of these materials, the dipyridyl behaves as a ligand, charge balancing cation, and/or templating species, respectively. Presented will be synthesis and structural systematics of the three novel uranium structures.



Sorption Properties of Pure Silica ITQ-13

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The synthesis and structure of the pure silica zeolite ITQ-13 was recently reported by Bix et al.¹ and Corma et al.². ITQ-13 has a three-dimensional, 9-ring [100], 10-ring [010] and 10-ring [001] channel structure having similarities to the pore system of ZSM-5. As the ring sizes are 5-9% smaller than those of ZSM-5, the diffusion coefficients (D's) are expected to be lower. However, the thin platelet morphology of the material studied resulted in very rapid adsorption rates preventing accurate measurement of D; no comparison of the D's for these two zeolites could be made. The adsorption properties of propane, n-butane, n-hexane, 2,2-dimethylbutane, benzene, toluene, p-xylene and o-xylene have been measured and will be presented.

(1) T. Boix, M. Pucha, M. A. Cambor, A. Corma, U.S. Pat. 6,471,941 B1 2000.

(2) Corma, A.; Puche, M.; Rey, F.; Sankar, G.; Teat, S. J. *Angew. Chem., Int. Ed.* **2003**, *42*, 1156.



Simulating Equilibration of Microwave Heated Zeolite Systems

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Microwave (MW) heating of zeolites has recently become a new target for researchers in nanoscience and engineering. This interest is fueled principally by experiments showing new and interesting energy efficiencies and selectivities for reactions and separations performed in zeolites under the influence of MW radiation. To approach an atomistic description of this experimental work, we have modeled the relaxation dynamics of MW-heated steady states for two zeolite systems by performing molecular dynamics simulations. We have studied dynamics in two FAU-type zeolites: NaY and methanol in siliceous-Y, where MW energy is directly absorbed by Na cations and methanol molecules, respectively. By applying a MW field and using an appropriate thermostat, we generated MW-heated steady states. Once these steady states were reached, we turned off both the MW field and the thermostat to let the system equilibrate. We have found that rather than a single exponential, subsystem temperatures must be fitted to a double exponential function. Short-time decay constants for the thermal relaxation strongly depend on the initial conditions, namely the MW field intensity and the thermostat target temperature; while the long-time decay constants do not. These long-time decay constants, which control the lifetimes of MW-generated athermal effects, were found to be surprisingly long considering typical vibrational frequencies in zeolite-guest systems. We discuss the physical origin of these characteristics by analyzing kinetic energy correlation functions.



Microporous Metal Organic Material Suitable for Separation of Hydrocarbons?

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A new microporous metal coordination material (MMOM), $[\text{Cu}(\text{hfipbb})(\text{H}_2\text{hfipbb})_{0.5}]$ [H_2hfipbb = 4,4'-(hexafluoroisopropyl idene)bis(benzoic acid)] (**1**) having unique channels along the [010] direction and a pore volume of 0.070 cc/g has demonstrated ~1 wt % of hydrogen uptake at room temperature and 48 atm. In addition, it exhibits interesting and subtle separation properties which are the focus of this presentation. Experiment shows that structure **1** adsorbs propene and propane rapidly but does not adsorb butane or higher normal or branched hydrocarbons. In contrast, all zeolites that adsorb propane and higher paraffins do not have a fixed carbon number cutoff for adsorption. This unusual property is attributed to the unique shape of the 1D channels. These channels are composed of alternating columns of cages 7.3Å in length and necks of 3.4 Å in diameter. The size of these cages and necks are the determining factors for the observed selectivity of gas adsorption. Simulation results from Cerius2 are in agreement with the experimental data.