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To accompany the 1992 Renewal Proposal of this Grant.

CHEMISTRY OF BIMETALLIC AND ALLOY SURFACES

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I. INTRODUCTION

In this report, a brief review is presented of accomplishments during our current funding period (DE-FG03-90ER14117). This grant was awarded on June 1, 1990, and was an extension of funding from DOE that began in 1986. In the past two years, we have 21 papers either published or in press in refereed journals, and a few more submitted. These are discussed briefly in Section II and listed in the Bibliography. In addition, there are a number of papers in preparation and ongoing research projects. Some of these are briefly summarized in Section III.

Specific Project Objectives

Surface science experiments in UHV were carried out to explore the chemisorption and reactions of several small molecules (CO, H_2, and O_2) and hydrocarbons (C_2H_4 and C_2H_2) on well-characterized bimetallic and alloy surfaces. We obtained basic data for the adsorption and decomposition of these molecules on single-crystal surfaces which had been characterized using Auger (AES) and photoelectron spectroscopy (UPS and XPS) and low energy electron diffraction (LEED). The structure and bonding of adsorbed molecules were studied by vibrational spectroscopy using high resolution electron energy loss spectroscopy (HREELS) and by temperature programmed desorption (TPD). Carefully chosen bimetallic surfaces, primarily Pt(111) and Ni(100) surfaces that contained another metallic element, such as K, Bi, or Sn, were systematically studied in order to gain a better fundamental understanding of the role of electronic and geometric effects in modifying the chemistry of these surfaces. We established correlations between changes in chemisorption bond strengths, adsorption site distributions, and hydrocarbon fragment stability and reactivity with the geometric and electronic structure of the metal atoms on the bimetallic surface. Direct comparison of the influence of Bi adatoms on Pt(111) with that of K adatoms on the chemistry of ethylene and hydrogen allowed us to separate which effects of K promotion were due to to site-blocking and which were due to electronic structure changes.

II. SUMMARY OF OVERALL PROGRESS

A. Highlights of Recent Research Accomplishments

- *A Method for Estimating Surface Reaction Energetics: Application to the Mechanism of Ethylene Decomposition on Pt(111)* [2].

A semi-empirical GVB method for estimating surface thermochemistry of adsorbed hydrocarbons was developed with Prof. Emily Carter of UCLA. I believe that this method will have an enormous impact on our ability to construct "zeroth order" potential energy diagrams for understanding surface reaction energetics. This method was applied to the ethylene dehydrogenation reaction on unpromoted and K-promoted Pt(111), and is currently being used in a number of other hydrocarbon reactions.

- *Carbon Auger Line Shapes for the Adsorption and Decomposition of Ethylene on Ni(100) and Carbon-Carbon Bonding in "Carbidic" Layers on Metals* [9,10].

Spectroscopic studies in collaboration with Prof. David Ramaker of George Washington Univ. have shown new insight into the nature of surface carbon on Ni(100). Adsorbed carbon has appreciable C-C bonding even in the "carbidic" state, and presumably exists as C_n oligomers to a large extent.

- *Surface Structure of Sn Deposited on Pt(111) by Low Energy Alkali Ion Scattering and Surface Science Examination of Sn Deposition on Pt(100)* [11,12,13].

The surface alloys that are formed from deposition of Sn on Pt(111) and Pt(100) have been characterized and studied concerning their chemisorption properties. Most importantly, a surface structural determination of Sn deposited on Pt(111) by Low Energy Alkali Ion Scattering (ALEISS) was carried out by in collaboration with Dr. Steve Overbury of Oak Ridge National Laboratory and Dr. Mark Paffett of Los Alamos National Laboratory. Surface structures resulting from the deposition and annealing of Sn on Pt(111) and exhibiting p(2 x 2) and $p(\sqrt{3} \times \sqrt{3})$-R30° LEED patterns were studied. Azimuthal and polar incident angle dependencies were measured for 500 and 1000 eV Li ions scattered from the clean and Sn covered surfaces. Shadowing and blocking effects adequately describe the single scattering from the clean Pt surface. The data support a structural model in which the Sn is incorporated into the Pt surface rather than existing as an overlayer. Analysis of the Sn angle dependence indicates that the Sn is not co-planar with the Pt but is protruding .022 ± .05 nm above the surface. The results are critical for interpreting the chemistry of these surfaces and represent an important advance in our understanding of metal alloy surface structure in their own right.

- *Chemisorption of CO, H_2, and O_2 on Ordered Sn/Pt(111) Surface Alloys* [6].

The chemisorption of CO, H_2, O_2 and C_2H_4 on ordered Pt-Sn surface alloys has been investigated. No ethylene dehydrogenation occurs on the alloy surfaces, in stark contrast to the facile dehydrogenation that occurs on Pt(111) surfaces. Alloying with Sn causes only slight decreases in the CO desorption peak temperature compared to Pt(111). HREELS indicates the atop-bonded CO is the most strongly adsorbed species on both ordered alloy surfaces, as on Pt(111), and that both atop and bridge sites are populated for saturation CO coverage on both ordered alloy surfaces. No dissociative H_2 adsorption is observed on either the p(2x2) or $(\sqrt{3} \times \sqrt{3})$R30° Sn/Pt ordered alloy surfaces. However, H atoms will adsorb on both surfaces. H_2 desorption from the H adlayers occurs with a slightly higher peak temperature than on Pt(111). In addition to this shifted desorption peak, another low temperature H_2 desorption state is observed for the $(\sqrt{3} \times \sqrt{3})$R30° Sn/Pt alloy surface. No molecular or dissociative O_2 adsorption is observed on either of the two ordered alloy surfaces over the range 100-600 K. This suppression of chemisorption for the alloy surfaces is in contrast to increased oxygen uptake by unalloyed Sn overlayers on

Pt(111) and the difference is due to changes in the electronic structure of the surface that accompany alloy formation. These changes have been examined using UPS for the ordered Sn/Pt(111) alloys.

- *Influence of Potassium on the Adsorption of H_2 on Pt(111)* [17].

The influence of potassium adatoms on the adsorption and desorption kinetics of hydrogen on the Pt(111) single-crystal surface was studied. Dissociative H_2 sticking probabilities were measured as a function of potassium coverages. Even small amounts of potassium drastically reduce the sticking probability for H_2 on Pt(111). For example, when $\theta_K \geq 0.04$ the sticking probability of H2 at 100 K has been reduced by more than a factor of 10. We also find that the role of an adsorbed precursor state in H_2 adsorption on Pt (111) is decreased by the presence of K, and the activation energy for dissociative adsorption of H_2 is increased. Hydrogen adatoms adsorbed on the K modified surface are thermally stabilized compared to Pt(111). The peaks observed during H_2 TPD occur with peak temperature up to 150 K higher for the K modified surface than for equivalent hydrogen coverages on Pt(111). We explain these observations by a simple Pt atoms, due to charge transfer from K to Pt. This has two effects, (i) to destabilize the bonding of H_2 to the surface and (ii) to stabilize the bonding of $H_{(a)}$ to the surface. A decrease in the Pt-$H_{2(a)}$ interaction caused by K lowers the initial sticking probability, inhibits the role of an adsorbed H_2 precursor in the adsorption kinetics, and causes an increase in the activation energy for dissociative adsorption H_2. These effects dominate over the possible effects of the increased Pt-H bond strength in enhancing the kinetics for H_2 adsorption.

- *Effects of Surface Modifiers (K(a), O(a), and H(a)) on the Adsorption Kinetics of CO on Pt(111)* [20].

The sticking coefficient, S, of CO on clean and K-, O-, and H-modified Pt(111) surfaces has been measured directly using a simple kinetic uptake method, as a function of CO and modifier coverage and surface temperature. A simple method is also introduced to determine the coverage-dependent desorption energy from these measurements without the need to know the preexponential factor or desorption order for those systems where S is only a function of coverage or only weakly dependent on temperature. The major influence of adsorbed K on the initial sticking coefficient of CO on Pt(111) at 320 K is site blocking, and the magnitude of this effect correlates well with the size of the adsorbed K ion or atom. The shape of S as a function of CO coverage for low K coverages in the ionic regime is similar to that of CO on clean Pt(111). A dramatic change occurs for K coverages near or greater than 0.24 ML, where S passes through a maximum at about 1/3 of the saturation CO coverage and coincident CO and K desorption is observed. This behavior of S, which has not been seen before, can be fit quite adequately by a simple model that incorporates the reduced site blocking effects of K due to the CO-induced transition of K from a metallic neutral to an ionic state and the accompanying size change of K atoms. These results are best described by a coverage-dependent alkali-CO interaction. In additional studies, we find that adsorption of 0.25 ML O on Pt(111) has no effect on S at 100 K and at low CO coverages, and only the saturation CO coverage is reduced from 0.59 to 0.31 ML. In contrast, adsorbed H reduces not only the CO saturation coverage but also S even at low CO coverages.

- *Hydrocarbon Trapping and Condensation on Pt(111)* [21].

A direct, reflected beam method under ultrahigh vacuum conditions was used to measure the sticking coefficient of several small hydrocarbon molecules (methylcyclohexane, cyclohexane, toluene, benzene and methanol) on the clean and adsorbate-covered Pt(111) surfaces and on the molecular solid phases that can be formed at temperatures below that required for multilayer sublimation. We find that the sticking coefficient for all of these molecules on the clean Pt(111) surface and the molecular solid phase at 100 K is unity. This is in contrast to several previous reports in the literature. The simple, classical hard-cube model provides a useful way to understand this behavior.

- *Influence of Carbon on Cyclohexane Dehydrogenation on Pt(111) Surfaces* [23].

Surface carbon acts as a simple site blocker for the dehydrogenation of cyclohexane and the decomposition of benzene on Pt(111). At small carbon coverages, the decomposition of benzene is blocked more effectively than is cyclohexane dehydrogenation. Selectivity of cyclohexane dehydrogenation toward benzene formation is thus promoted. At high carbon coverage, cyclohexane dehydrogenation is also suppressed. The cyclohexane desorption peak at 165 K often seen in temperature programmed desorption (TPD) studies is shown to be due to a new desorption state formed by coadsorbed C or a decomposition intermediate.

- *A New Catalysis for Benzene Production from Acetylene under UHV Conditions: SnPt(111) Surface Alloys* [24].

The adsorption and reaction of acetylene on Pt(111), and the (2X2) and (√3X√3)Sn/Pt surface alloys were investigated with LEED, TPD and AES. The presence of Sn atoms at the surface of the (2X2) and (√3X√3)Sn/Pt surface alloys strongly suppressed the decomposition of acetylene to deuterium and adsorbed carbon. As a result, a new reaction path is opened on the Sn/Pt(111) surface alloys - **benzene formation**. Besides benzene desorption, we also observed butadiene desorption, which is obviously the intermediate product of benzene production. The (√3X√3)Sn/Pt-surface shows the highest activity and selectivity for the formation of benzene and the intermediate - butadiene. Following C_2D_2 adsorption at 110 K, LEED shows a faint (2X2) pattern on the Pt(111) surface. After saturation dosing of acetylene on the (2X2)Sn/Pt surface at 110 K we find a large increase in the (2X2) LEED pattern intensity. This implies that an acetylene (2X2)-substructure also forms on the (2X2)Sn/Pt-surface.

B. Project Personnel

Students Contributing to the DOE Project:

1. Mr. John Heitzinger, a fifth year graduate student (B.S. Univ. Wisconsin-Stevens Point), designed and constructed a collimated gas beam doser in one of our vacuum chambers. He was also responsible for setting up the main XPS system we use. He received his Ph.D. this summer and is leaving USC to take a postdoctoral position in the Science and Technology Center in Austin, TX.

2. Dr. George Kastanas, a postdoctoral fellow who received his Ph. D. in Chemical Engineering in 1989 working with Prof. J. Schwank at Michigan, (thesis title: "Novel catalytic materials for methane activation and selective oxidation of hydrocarbons"), built the small volume reaction cell used for atmospheric pressure reaction kinetics studies of unsupported Pt catalysts. He installed a HP-5890 gas chromatograph (GC) for these studies and worked on the calibration of the GC for all of the hydrocarbon reactants and products related to cyclohexane conversion to benzene.

His postdoctoral appointment in my group ended this summer, and he is pursuing a new project at USC modeling combustion kinetics.

3. Mr. Armen Avoyan, a second year graduate student (B.S. Moscow Institute of Steel and Alloys), has been working on our HREELS instrument. His projects include detailed measurements of the desorption kinetics of K from Pt(111), and studies of cyclohexane, benzene, and acetylene adsorption on K-modified Pt(111).

4. Mr. John Peck, a first year graduate student (B.S. American University), has been working this summer on our XPS, TPD, and adsorption kinetics instrument. He has started measuring adsorption rates of hydrocarbons on clean Pt(111) and ordered surface alloys of Sn/Pt.

4. Dr. Liqiang Jiang, a postdoctoral fellow who received his Ph. D. in Physics in 1990 working with Prof. M. Strongin at Queens College of CUNY, (thesis title: "Growth and electronic properties of selected bimetallic interfaces"), calibrated the collimated gas beam doser, measured the sticking probability of CO, and initiated the experiments measuring adsorption rates of hydrocarbons on clean and chemically modified Pt(111).

5. Dr. Chen Xu, a postdoctoral fellow who received his Ph. D. in Chemistry in 1991 working with Prof. H.-J. Freund at Ruhr-University Bochum FRG, (thesis title: "Adsorption of CO, NO, CO_2, NO_2 and H_2O on Cr_2O_3 (111)/Cr(110)"), has initiated a number of experiments measuring adsorption rates of hydrocarbons on clean Pt(111) and ordered surface alloys of Sn/Pt.

Collaborations

Formally, there are no other collaborators on the project; there is no Co-PI nor subcontracts. However, we have a very interactive group and several other scientists from around the country have participated with us in some of the most interesting work. These informal collaborations take advantage of the individual expertise of those involved and have generated exciting new science, resulting in a number of publications. A list of coauthors on papers acknowledging DOE support from 1990 onward is given below:

Dr. M. T. Paffett, Dr. A. D. Logan, and Dr. R. J. Simonson	Los Alamos National Laboratory
Dr. S. H. Overbury and Dr. D. R. Mullins	Oak Ridge National Laboratory

Prof. J. L. Gland	University of Michigan, Ann Arbor
Dr. D. A. Fischer and Dr. J. Colbert	Brookhaven National Laboratory
Prof. E. A. Carter	University of California, Los Angeles
Prof. J. L. Falconer	University of Colorado, Boulder
X.-L. Zhou, P. M. Blass, and Prof. J. M. White	University of Texas, Austin
Dr. J. E. Houston, Dr. J. A. Kelber, and Dr. J. W. Rogers, Jr.,	Sandia National Laboratories
Prof. F. L. Hutson and Prof. D. E. Ramaker,	George Washington Univ. & NRL

Former Students and Postdocs at CU:
S. C. Gebhard, Dr. M. E. Jones, D. Parker, B. A. Banse, R. G. Windham, R. J. Smith, K. A. Magrini, D. H. Parker

III. DESCRIPTION OF ONGOING RESEARCH

Clearly, the most important activity for us is to continue our studies of hydrocarbon chemistry on ordered Sn/Pt alloy surfaces that can be formed by vapor depositing Sn on single crystal Pt samples. *The research plan for this activity is laid out in the accompanying Renewal Proposal.* The atomic structures of the Sn/Pt(111) surfaces have been solved, while those of the Sn/Pt(100) surfaces still require investigation. Chemisorption studies are revealing important details about how Sn influences adsorption and desorption kinetics, structure and bonding of hydrocarbon intermediates, and the thermochemistry of hydrocarbon conversion reactions on these surfaces. By comparison of similar studies on Sn/Pt(100) and Sn/Pt(111), these unique surface alloys may allow us to probe the actual type and number of sites required for chemical reactions at the surface, as opposed to simply the ensemble size or "Pt area" requirements.

In addition, several studies are underway that address important issues raised in our previous work on K- and C-modified Pt(111) or Ni(100) surfaces. In many cases, papers are now being written on completed experiments. For example, we are completing our studies of ethylene adsorption on Pt(111) and K-modified Pt(111). This involves evaluating further the site blocking effects in K coadsorption by detailed comparison to Bi data and modeling studies of Bi and ethylene coadsorption. We have completed a number of experiments on ethylene and acetylene adsorption and decomposition on Ni(100), and the use of coadsorbed bismuth to determine adsorption and reaction ensemble size requirements of these hydrocarbons on this surface. This evaluation first required measurements of the structure and bonding of Bi adatoms on Ni surfaces. In addition, CO adsorption on Bi/Ni(100) surfaces and Bi adsorption on CO/Ni(100) surfaces was studied.

Finally, we are scaling back our surface chemistry studies of model HDS and HDN catalysts. We have made some progress in vapor-depositing cobalt and palladium on Mo(100) surfaces, but we are spread a little thin now and we will just try to wrap up this work. We are also trying to conclude an investigation of CO chemisorption on Ag/Cu(110) surfaces in collaboration with Dr. Tom Taylor of Los Alamos National Laboratory .

Selected Examples of Papers in Preparation:

A. Adsorption and Growth Modes of Bi on Ni(100)

The surface structure and growth mechanism of vapor deposited Bi on Ni(100) has been investigated by Auger electron spectroscopy (AES), temperature programmed desorption (TPD), low-energy electron diffraction (LEED), energy loss spectroscopy (ELS) and UV photoelectron spectroscopy (UPS). At 500 K Bi growth proceeds via a layer plus island (Stranski-Krastanov) growth mode. ELS data are consistent with this mechanism as indicated by the disappearance of the Ni surface plasmon at low Bi coverages. Desorption of the first monolayer is characterized by a coverage dependent desorption activation energy which varies from 70 to 57 kcal mol^{-1}. Multilayer coverages desorb with zero-order kinetics and E_{des} = 48 kcal mol^{-1}. LEED shows the gradual formation of a c(2x2) structure near monolayer coverage. Adsorbed Bi changes the work function of the Ni surface by 1.0 eV at monolayer coverage. The change in work function, $\Delta\phi$, as a function of coverage indicates little charge transfer between Bi and Ni, and an initial dipole moment of only -0.5 D. A comparison of this system to Bi on Pt(111), in which Bi has been used as a model inert site-blocking agent, indicates that Bi modifies the electronic structure Ni(100) even less than in the case of Pt(111). Therefore, Bi adatoms may allow useful probing of reaction ensemble requirements on Ni surfaces .

B. Comparisons of Acetylene and Ethylene Decomposition on Ni(100): An Explanation of the Apparent Structure Sensitivity of Ni Surfaces.

Acetylene and ethylene dehydrogenation are structure sensitive reactions on nickel. These reactions were examined on Ni(100) using Temperature Programmed Desorption (TPD) and High Resolution Electron Energy Loss Spectroscopy (HREELS). Vibrational spectra using HREELS after saturation C_2H_2 and C_2H_4 exposures made at 320 K on Ni(100) indicate that different hydrocarbon fragments are formed in each case. Hydrogen TPD after 320 K C_2H_2 and C_2H_4 saturation exposures onto clean Ni(100) and H2 TPD after small C_2H_2 and C_2H_4 exposures onto carbon adatom precovered Ni(100) were also investigated. These results show that the structure sensitivities of C_2H_2 and C_2H_4 dehydrogenation on nickel are not due to "new" species being formed, but rather due to differences in the decomposition kinetics that take place as a function of the hydrocarbon coverage. Differences in how these molecules initially chemisorb to the various nickel crystal faces control this coverage and ultimately the observations of structure sensitivity.

C. Adsorption and Decomposition of Acetylene on Ni(100).

Acetylene dehydrogenation on Ni(100) has been investigated by means of Temperature Programmed Desorption (TPD) and High Resolution Electron Energy Loss Spectroscopy

(HREELS). High temperature H_2 desorption states are observed during TPD at high C_2H_2 coverages that are not observed at low C_2H_2 coverage. Vibrational spectroscopy (HREELS) has been used to study C_2H_2/Ni(100) at various coverages on both clean and carbon adatom precovered Ni(100) surfaces. At low coverage on clean Ni(100), decomposition follows the scheme: $C_2H_{2(ads)} \rightarrow CCH_{(ads)} \rightarrow C_{(ads)}$; whereas at high coverage, the reaction takes place according to the scheme: $C_2H_{2(ads)} \rightarrow CCH_{(ads)} \rightarrow CH_{(ads)} \rightarrow C_{(ads)}$. These results show an increase in the activation energy for CH bond breaking occurs as C_2H_2 coverage increases. This is supported by both TPD and HREELS results for small coverages of C_2H_2 on carbon adatom pre-covered Ni(100), as well as studies of 320 K saturation C_2H_2/Ni(100).

IV. BIBLIOGRAPHY

A. Recent (1990-current) Publications that Acknowledge DOE Support:

1. "Coadsorption of Ethylene and K on Pt(111). 2. Influence of K on the Decomposition of Ethylene", R. G. Windham and B. E. Koel, *J. Phys. Chem.*, **94**, 1489-1496 (1990).

2. "A Method for Estimating Surface Reaction Energetics: Application to the Mech. of Ethylene Decomposition on Pt(111)", E.A. Carter and B.E. Koel, *Surface Sci.*, **226**, 339-357 (1990).

3. "Chemisorption of High Coverages of Atomic Oxygen on the Pt(111), Pd(111), and Au(111) Surfaces", D. H. Parker and B. E. Koel, *J. Vac. Sci. Technol.*, **A 8**, 2585-2590 (1990).

4. "Temperature Programmed Desorption of Bi on Ni(100)", M. E. Jones, J. M. Heitzinger, R. J. Smith, and B. E. Koel, *J. Vac. Sci. Technol.*, **A 8**, 2512-2516 (1990).

5. "Interaction of Dimethylamine with Clean and Partially Oxidized Copper ", J.A. Kelber, J.W. Rogers, Jr., B.A. Banse, and B.E. Koel, *Appl. Surface Sci.*, **44**, 193-204 (1990).

6. "Chemisorption of CO, H_2, and O_2 on Ordered Sn/Pt(111) Surface Alloys", M. T. Paffett, S. C. Gebhard, R. G. Windham, and B. E. Koel, *J. Phys. Chem.*, **94**, 6831-6839 (1990).

7. "Hydrogen-Induced Low Temperature CO Displacement from Pt(111)", D. H. Parker, D. A. Fischer, J. Colbert, B. E. Koel, and J. L. Gland, *Surface Sci.*, **236**, L372-L376 (1990).

8. "Methyl Chloride and Trichlorosilane Adsorption on Cu(110)", K. A. Magrini, S. Gebhard, F E. Koel, and J. L. Falconer, *Surface Sci.*, **248** 93-103 (1991).

9. "Spectroscopic Evidence for Carbon-Carbon Bonding in "Carbidic" Layers on Metals", F. L. Hutson, D. E. Ramaker, and B. E. Koel, *Surface Sci.*, **248**, 104-118 (1991).

10. "Interpretation of the Carbon Auger Line Shapes for the Adsorption and Decomposition of Ethylene on Ni(100)", F. L. Hutson, D. E. Ramaker, B. E. Koel, and S. C. Gebhard, *Surface Sci.*, **248**, 119-133 (1991).

11. "Structure of Metal Overlayers by Low Energy Alkali Ion Scattering: Cu/Ru (0001) and Sn/Pt (111)", S. H. Overbury, D. R. Mullins, M. T. Paffett, and B. E. Koel, in Structure of Surfaces III, Springer Series in Surface Science, Proceed. of ICSOS III, Milwaukee, 1990, M. A. Van Hove and S. Y. Tong, (Eds.), (Springer-Verlag, New York), in press.

12. "A Multitechnique Surface Science Examination of Sn Deposition on Pt(100)", M. T. Paffett, A. D. Logan, R. J. Simonson, and B. E. Koel, *Surface Sci.*, **250**, 123-138 (1991).

13. "Surface Structural Determination of Sn Deposited on Pt(111) by Low Energy Alkali Ion Scattering", S. H. Overbury, D. R. Mullins, M. T. Paffett, and B. E. Koel, *Surface Sci.*, **254**, 45-57 (1991).

14. "A Vibrational Study of Borazine Adsorbed on Pt(111) and Au(111) Surfaces", R. J. Simonson, M. T. Paffett, M. E. Jones, and B. E. Koel, *Surface Sci.*, **254**, 29-44 (1991).

15. "High Resolution Electron Energy Loss Spectroscopy (HREELS)", B. E. Koel, in Encyclopedia of Materials Characterization, Vol. on Instrumental Analytical Techniques for Surface Analysis, C. Evans, R. Brundle, and S. Wilson, Eds., (Butterworth, 1992), in press.

16. "Hydrogen-Induced CO Displacement from Pt(111): An Isothermal Kinetic Study", D.H. Parker, D.A. Fischer, J. Colbert, B.E. Koel, and J.L. Gland, *Surface Sci.*, **258**, 75-81 (1991).

17. "Influence of Potassium on the Adsorption of H_2 on Pt(111)", S. C. Gebhard and B. E. Koel, *J. Phys. Chem.*, **96**, 7056-7063 (1992).

18. "Low Energy Electron Induced Chemistry: CH_3Cl on Ag(111)", X.-L. Zhou, P. M. Blass, B. E. Koel, and J. M. White, *Surface Sci.*, in press.

19. "Low Energy Electron Induced Chemistry: C_2H_5Cl on Ag(111)", X.-L. Zhou, P. M. Blass, B. E. Koel, and J. M. White, *Surface Sci.*, in press.

20. "Effects of Surface Modifiers (K(a), O(a), and H(a)) on the Adsorption Kinetics of CO on Pt(111)", L. Q. Jiang, B. E. Koel, and J. L. Falconer, *Surface Sci.*, in press.

21. "Hydrocarbon Trapping and Condensation on Pt(111)", L. Q. Jiang and B.E. Koel, *J. Phys. Chem.*, in press.

22. "Thermal Decomposition of Alkenes, Alkynes, and Dienes at High Temperatures on Rh(111)", J.E. Crowell, B.E. Bent, B.E. Koel, C.M. Mate, and G.A. Somorjai, *J. Phys. Chem.*, submitted.

23. "Influence of Carbon on Cyclohexane Dehydrogenation on Pt(111) Surfaces", C. Xu and B.E. Koel, *J. Catal.*, submitted.

24. "A New Catalysis for Benzene Production from Acetylene under UHV Conditions: SnPt(111) Surface Alloys", C. Xu, J.W. Peck, and B.E. Koel, *J. Amer. Chem. Soc.*, submitted.

B. Invited Talks at Meetings, Invited Lectures at Universities and Laboratories, and Contributed Papers at Technical Meetings:

The following is a list of recent (1990-current) invited talks and lectures and contributed papers at scientific meetings which specifically discussed our results from DOE-funded projects and acknowledged DOE support.

Invited Talks at Meetings:

3/90	"Chemisorption and Reaction on Metal Alloy Surfaces", APS March Meeting, Division of Condensed Matter Physics, Symposium on Atomic and Electronic Structure of Alloy Surfaces, Anaheim
6/90	"Adsorption/Desorption on Alloy Surfaces", DOE Surface Studies Conference, 16th, Golden
6/90	"Chemisorption and Reaction on Metal Alloy Surfaces", Symposium on Frontiers of Surface Chemistry, Catalysis Research Center, Hokkaido University, Sapporo, Japan
10/91	"Adsorption and Desorption Kinetics of Methylcyclohexane and Toluene on Potassium and Carbon Modified Pt(111) Surfaces" 18th Annual Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS)/13th Pacific Conference on Chemistry and Spectroscopy and 27th Western Regional ACS Meeting, Symposium on Reactions at Surfaces, Anaheim
3/92	"Chemistry of Bimetallics and Alloys: Ordered Sn/Pt Surfaces" Eighth DOE/BES Heterogeneous Catalysis and Surface Chemistry Meeting, Santa Monica
5/92	"Chemistry of Bimetallic and Alloy Surfaces" DOE/BES Catalysis Research Review, Bethesda

Invited Lectures at Universities and Laboratories:

2/90	"Adsorption and Reaction on Bimetallic Surfaces" Amoco Oil Company, Naperville, IL
2/90	"Recent Advances in Establishing Structure-Reactivity Relationships in Surface Chemistry Ford Motor Company, Dearborne, MI
2/90	"Recent Advances in Establishing Structure-Reactivity Relationships in Surface Chemistry Dow Chemical Company, Midland, MI
2/90	"Separation of Electronic and Geometric Effects in Bimetallic Surface Chemistry and Catalysis" Michigan Catalysis Society, Detroit, MI

2/90	"Recent Advances in Establishing Structure-Reactivity Relationships in Surface Chemistry California Institute of Technology, Pasadena, CA, Department of Chemistry
5/90	"Recent Advances in Establishing Structure-Reactivity Relationships in Surface Chemistry Columbia University, New York, NY, Department of Chemistry
5/90	"Recent Advances in Establishing Structure-Reactivity Relationships in Surface Chemistry Rutgers University, New Brunswick, NJ, Department of Chemistry
5/90	"Recent Advances in Establishing Structure-Reactivity Relationships in Surface Chemistry Princeton University, Princeton, NJ, Department of Chemistry
5/90	"Recent Advances in Establishing Structure-Reactivity Relationships in Surface Chemistry General Motors Research Laboratories, Warren, MI
11/90	"Chemistry of Bimetallic and Alloy Surfaces" University of California, Irvine, CA, Department of Chemistry
5/92	"Chemistry of Bimetallic and Alloy Surfaces" University of California, San Diego, Department of Chemistry

Contributed Papers at Meetings:

Adsorption and Decomposition of Borazine on Pt(111) and Au(111)
B. E. Koel, R. J. Simonsen, M. T. Paffett, M. Jones, M. W. Trenary and R. T. Paine
Gordon Conference on Electronic Materials, Ventura, CA, February, 1990

The Influence of Potassium on the Adsorption of Hydrogen on Pt(111)
S. C. Gebhard, R. G. Windham, and B. E. Koel,
16th DOE Surface Studies Conference, Golden, CO, June, 1990

Vibrational Spectroscopy of Borazine Adsorption on Pt(111)
R. J. Simonsen, **M. T. Paffett**, and B. E. Koel,
16th DOE Surface Studies Conference, Golden, CO, June, 1990

Structure of Metal Overlayers by Low Energy Alkali Ion Scattering: Cu/Ru (0001) and Sn/Pt (111)
S. H. Overbury, D. R. Mullins, M. T. Paffett, and B. E. Koel,
3rd International Conference on Structure at Surfaces (ICSOS III), Milwaukee, WI, 1990.

CO Displacement and Repulsive Interactions on the Pt(111) Surface
D. H. Parker, D. A. Fischer, J. Colbert, B. E. Koel, and J. L. Gland,
Chemistry at Surfaces Meeting, Irvine, CA, October, 1990

Growth Modes and Chemistry of Bismuth on Ni(100)
J. M. Heitzinger and B. E. Koel,
Chemistry at Surfaces Meeting, Irvine, CA, October, 1990

Vibrational Spectroscopy of Borazine Adsorption on Pt(111)
R. J. Simonsen, M. T. Paffett, B. E. Koel, and M. Trenary,
37th National Symposium of the American Vacuum Society, Toronto, Canada, October 1990

Influence of Potassium on the Adsorption of H_2 on Pt(111)
S. C. Gebhard, R. G. Windham, and B. E. Koel,
12th North American Meeting of the Catalysis Society, Lexington, KY, May, 1991

Effects of $K_{(a)}$ on the Adsorption Kinetics of CO on Pt(111)
L. Q. Jiang, B. E. Koel, and J. L. Falconer,
California Catalysis Society, Fall Meeting, Santa Barbara, CA, November, 1991

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