

## Final Report for DOE OBES Grant

**GRANT NUMBER: DE-DG02-06ER15785**

**GRANT TITLE:**

**Support of 5<sup>th</sup> the International Workshop on Oxide Surfaces (IWOX-V)**

**PI: Charles T. Campbell, University of Washington**

**Budget period: 7/1/06-5/31/07.**

The 5<sup>th</sup> International Workshop on Oxide Surfaces (IWOX-V) was held at Granlibakken Conference center in Lake Tahoe, CA, January 7-12. The total attendance was ~90. The breakdown of attendees by country is as follows:

USA	41
Germany	18
Japan	7
UK	5
Italy	5
France	4
Austria	3
Denmark	3
Cech. Repub.	1
Ireland	1
New Zealand	1
India	1

The technical program (see attached) included oral sessions on the electronic and magnetic properties of oxide surfaces, surface and interface structure, advances in theory, surface defects, thin film oxides on metals and on oxides, thin film metals on oxides, surface photochemistry, surface reactivity, and interactions with water. Two evening poster sessions had similar themes. As in previous years, the program stimulated significant interest and discussion among the attendees.

The invited speakers and their institutions and topics are listed below.

Thomas Risse (Fritz Haber Institute) – Development of ESR to study point defects on oxide surfaces, in combination with STM and STS.

Russel Egdell (Oxford University) – Relationship between surface properties and the electronic structure in metal oxides, particularly epitaxial oxide films.

John Freeland (ANL) -- x-ray scattering and x-ray magnetic circular dichroism of manganite surfaces.

Nick Harrison (Imperial College – London)

Yuji Matsumoto (Tokyo Inst. of Technology) – photocatalysis and structure on oxide surfaces.

Zdenek Dohnalek (PNNL) – reactivity of metal particles on oxide surfaces.

Hiroshi Onishi (Kobe University) – STM investigations of photochemical processes on oxide surfaces with small metal particles.

Remi Lazzari (INSP, Paris) -- Growth of metal clusters on oxide surfaces by GISAXS and GIXRD.

Svetlozar Surnev (University of Graz, Austria) -- metal supported NiO and MnO<sub>x</sub> nanostructures.

Gaetano Granozzi (University of Padova, Italy) – experimental investigations of TiO<sub>x</sub> films on Pt (111).

Marija Gajdardziska-Josifovska (University of Wisconsin at Milwaukee) – TEM and theoretical investigations of polar oxide surfaces and interfaces.

Kevin Rosso (PNNL) -- single crystal mineral (iron oxides) dissolution.

The local expenses (food and lodging, \$918 per person) for Dohnalek, Freeland, Harrison, Gajdardziska-Josifovska, Lazzari, Onishi, Risse, and Surnev were covered by BES funds. In addition, partial reimbursement for travel (\$328 per person) was given to Freeland and Gajdardziska-Josifovska. (See budget details below.)

Nine Ph.D. students competed for the Best Student Presentation Prize, a new prize instituted in 2007 for the first time. The prize consists of a certificate and \$500. The winner, selected by a multinational panel of judges, was Stefan Torbrügge of Universität Osnabrück, Germany. This money was provided by Elsevier.

IWOX-VI will be held at January 18-23, 2009 in Schaldming Austria, and will be chaired by Falko Netzer of Graz University, Vienna. IWOX-VII will be held in the winter of 2010 in Japan, and will be chaired by Hiroshi Onishi and Yuji Matsumoto of Kobe University and the Tokyo Institute of Technology, respectively. Despite the biannual schedule we have used since the inception of IWOX, it was decided to hold IWOX-VII one year after IWOX-VI in order to eliminate an ongoing schedule conflict between IWOX and the Water on Oxides Gordon Conference, which is held biannually in February, and has coincided with IWOX since the inception of the latter. Some academics have reported that they cannot attend both conferences when they are so close together due to teaching responsibilities. By staggering the meetings in this way, more individuals should be able to attend both.

### Budget Details

<u>Invited Speaker</u>	<u>lodging/meals</u>	<u>airfare</u>	<u>total</u>
Zdenek Dohnalek	\$918	0	\$918
Nick Harrison	\$918	0	\$918
Remi Lazzari	\$918	0	\$918
Hiroshi Onishi	\$918	0	\$918
Thomas Risse	\$918	0	\$918
Svetlozar Surnev	\$918	0	\$918
John Freeland	\$918	\$328	\$1246
<u>Marija Gajdardziska-Josifovska</u>	\$918	\$328	<u>\$1246</u>
Grand total			\$8000
Total funds received from DOE-BES			\$8000
Funds remaining			0

## IWOX - V Technical Program

### Sunday, Jan. 7

5:00 -- 7:00	Registration
7:00 – 8:00	Dinner
8:00 – 10:00	Evening reception

### Monday, Jan. 8

6:30 – 8:00	Breakfast
7:00 – 8:00	Late Registration
8:15 – 8:30	Welcome and Opening Remarks

#### **Oral Session 1 Electronic Structure of Oxide Surfaces and Epitaxial Films (S.A. Chambers)**

8:30 – 9:10	<i>R.G. Egdell</i> - Electronic Structure and Surface Properties of Lead Oxides
9:10 – 9:30	<i>H. Pfnür</i> - Epitaxial Growth, Stoichiometry and Electronic Properties of an Alternative Gate Oxide: Lattice Matched SrO/BaO Mixtures on Si(100)
9:30 – 9:50	<i>S.H. Cheung</i> - Fundamental studies of N incorporation and Electronic Structure in N-doped TiO <sub>2</sub> Grown by Plasma Assisted Molecular Beam Epitaxy
9:50 – 10:10	<i>W. Widra</i> – Layer-resolved Electronic Structure of NiO and CoO Thin Films on Ag(001): An STM, STS and DFT Study
10:10 – 10:40	Coffee break

#### **Oral Session 2 Magnetic and Electronic Properties of Oxide Surfaces (S.A. Chambers)**

10:40 – 11:20	<i>J.W. Freeland</i> - Unexpected Behavior at Oxide Surfaces and Interfaces
11:20 – 11:40	<i>V.E. Henrich</i> - Structure of the Fe <sub>3</sub> O <sub>4</sub> (100) Surface and its Interfaces with NiO (100) and CoO (100) Overlayers
11:40 – 12:00	<i>T.C. Droubay</i> - Epitaxial Ti-doped $\alpha$ -Fe <sub>2</sub> O <sub>3</sub> Hematite: Structure, Magnetism, and Conductivity
12:00 – 12:20	<i>J.-S. Kim</i> – Growth and Electronic Structure of Ultrathin NiO Films on Ag(001)
12:30 – 1:30	Lunch

#### **Oral Session 3 Oxide Surface and Interface Structure (B.D. Kay)**

1:30 – 2:10	<i>M. Gajdardziska-Josifovska</i> – From Polar Oxide Surfaces to Interfaces
2:10 – 2:30	<i>C.J. Hirschmugl</i> - Reconstructions of the Polar Oxide Surface MgO(111)
2:30 – 2:50	<i>X.-G. Gong</i> – Structure and Reactivities of Steps on Anatase TiO <sub>2</sub> (101)
2:50 – 3:10	<i>S. Gritschneider</i> – Order and Complexity in the Surface Structure of Alumina on Ni <sub>3</sub> Al(111)
3:10 – 3:40	Coffee break

#### **Oral Session 4 Advances in the Theory of Oxides (B.D. Kay)**

3:40 – 4:20	<i>N.M. Harrison</i> -- First Principles Simulation of Strongly Interacting Surfaces
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4:20 – 4:40	<i>M. Dupuis</i> -- Charge Transport in Photocatalysts: First Principles Characterization
4:40 – 5:00	<i>J. Graciani</i> - Interaction of Oxygen with TiN (001) and ScN (001): a DFT Study
5:00 – 5:20	<i>A. Fortunelli</i> - Density-functional Global Optimization of Metal Clusters Supported on the Regular and F <sub>s</sub> -defected MgO(100) Surface: A Study of their Structure and Diffusion
7:00 - 8:00	Dinner
8:00 – 10:00	<b>Poster Session I - Oxide Surface Structure, Electronic Properties, Photoresponse, Defect Structures, Reactivities, and the Student Poster Competition</b>

## Tuesday, Jan. 9

6:30 – 8:00	Breakfast
8:15 – 8:30	Information on skiing and other recreational activities
<b>Oral Session 5</b>	<b>Point Defects on Oxide Surfaces I</b> (M.A. Henderson)
8:30 – 9:10	<i>T. Risse</i> - Influence of Point Defects on the Properties of Deposited Metal Atoms and Clusters on Oxides: Au on MgO - A Case Study
9:10 – 9:30	<i>S. Torbrügge</i> - Evidence for Subsurface Oxygen Vacancy Arrays on Reduced CeO <sub>2</sub> (111)
9:30 – 9:50	<i>S. Fabris</i> - Oxygen Buffering at Reducible Oxide Surfaces: Interplay Between Vacancies, Electron Localization, and Adsorbate Mobility on Ceria
9:50 – 10:20	Coffee break
<b>Orals Session 6</b>	<b>Point Defects on Oxide Surfaces II</b> (M.A. Henderson)
10:20 – 10:40	<i>J. M. White</i> - Diffusion of Bridge-bonded Oxygen Vacancy on TiO <sub>2</sub> (110)
10:40 – 11:00	<i>G. Thornton</i> - Tracking the Reaction of O <sub>2</sub> and Surface Hydroxyl on TiO <sub>2</sub> (110) with Scanning Tunneling Microscopy
11:00 – 11:20	<i>G. H. Olesen</i> - Non-Contact Atomic Force Microscopy Study of TiO <sub>2</sub> (110) -Chemical Identification of Point Defects and Adsorbates
11:45 – 12:30	Lunch
12:30 – 8:00	Free time
8:00 – 9:00	Dinner

## Wednesday, Jan. 10

6:30 – 8:00	Breakfast
<b>Oral Session 7</b>	<b>Metals on Oxides I</b> (D.W. Goodman)
8:30 – 9:10	<i>R. Lazzari</i> - Watching Metal Nanoparticles Grow on Oxide Surfaces with X-ray scattering Techniques

- 9:10 – 9:30 *S. Schauerermann* - The Role of Metal-Support Interaction in Surface Reactions: Partial Oxidation and Catalytic Activity of Pd/Fe<sub>3</sub>O<sub>4</sub> Model Catalyst
- 9:30 – 9:50 *A. Hellman* – A First Principles Study of Ag/Al<sub>2</sub>O<sub>3</sub> Catalysts
- 9:50 – 10:10 *C.T. Campbell* – Thermodynamics of Surface Oxides and Metals on Oxides
- 10:10 – 10:40 Coffee break

**Oral Session 8**

**Metals on Oxides II** (D.W. Goodman)

- 10:40 – 11:20 *H. Onishi* - Charge Transfer at Metal-TiO<sub>2</sub> Interfaces
- 11:20 – 11:40 *S. Wendt* - Point-like Defect Sites and Bonding of Gold Nano-Particles on the TiO<sub>2</sub>(110) Surface
- 11:40 – 12:00 *T. Okawaza* - Electronic Properties of Au Nano-particles Supported on Stoichiometric and Reduced TiO<sub>2</sub>(110) Substrates
- 12:00 – 12:20 *W.-J. Chun* – STM Studies of Ni Clusters on a TiO<sub>2</sub>(110) Surface With a Wide Terrace
- 12:30 – 1:30 Lunch

**Oral Session 9**

**Oxides on Metals I** (H.J. Freund)

- 1:30 – 2:10 *G. Granozzi* - TiO<sub>x</sub> Nanostructures on Pt(111) and Pt(110) Substrates: a Combined LEED, Photoemission, STM and Theoretical Investigation
- 2:10 – 2:30 *D.W. Goodman* – Active Phases of Palladium Catalysts for CO Oxidation
- 2:30 – 2:50 *P. Varga* - The p(4 x4)-O Structure of Ag(111): No Surface Oxide
- 2:50 – 3:10 *S. Benedetti* - Structural and Morphological Characterization of Thin MgO Films on Mo(001)
- 3:10 – 3:40 Coffee break

**Oral Session 10**

**Oxides on Metals II** (H.J. Freund)

- 3:40 – 4:20 *S. Surnev* - Oxide Nanostructures on Metal Surfaces: Manganese Oxides on Pd(100)
- 4:20 – 4:40 *Ch. Hagendorf* - Structure and Vibrational Properties of Thin Mn Oxide Films on Pt(111) at Oxidizing and Reducing Conditions
- 4:40 – 5:00 *F.P. Netzer* - Low Dimensional Oxide Nanostructures on Stepped Metal Surfaces
- 5:00 – 5:20 *S. Shaikhutdinov* - Preparation and Atomic Structure of Well-ordered Silica and Aluminosilicate Films
- 7:00 - 8:00 Dinner
- 8:00 – 10:00 **Poster Session II - Oxides on Metals and Metals on Oxides**

**Thursday, Jan. 11**

- 6:30 – 7:50 Breakfast
- 7:50 – 8:00 Information on recreational activities and transportation to airport

**Oral Session 11**

**Adsorption and Reaction on Oxide Surfaces** (C.H.F. Peden)

- 8:00 – 8:20 *H. Idriss* - The Mineral Origin of Life. Surface Reactions of Oxides with Prebiotic Molecules.

- 8:20 – 8:40 *H. Kuhlenbeck* - Interaction of Methanol, Ethanol, and Propanol with  $V_2O_3(0001)$   
 8:40 – 9:00 *Y. Szanyi* - Model  $NO_x$  Storage Systems:  $NO_x$  Chemistry on  $BaO/\theta-Al_2O_3/NiAl(100)$   
 9:00 – 9:30 Coffee break

**Oral Session 12 Oxides on Oxides** (F.P. Netzer)

- 9:30 – 10:10 *Z. Dohnalék* - Structure and Catalytic Activity of Model Oxide Systems  
 10:10 – 10:30 *S. Bourgeois* - Growth of Tungsten Nanostructures on  $TiO_2(110)$  by Decomposition of Metalorganic Precursor. Reactivity Towards Oxygen.  
 10:30 – 10:50 *R.J. Lad* - Structure and Charge Transport of Thin Epitaxial  $Ag_2O$  Films Grown on Sapphire  
 10:50 – 11:10 *A. Stierle* - Oxidation of Pd Nanoparticles on Single Crystal Oxide Supports  
 11:45 – 12:30 Lunch  
 12:30 – 7:00 Free time  
 7:00 – 8:00 Reception  
 8:00 – 9:00 Dinner

**Friday, Jan. 12**

- 6:30 – 8:00 Breakfast

**Oral Session 13 Photochemistry at Oxides Surfaces** (H. Idriss)

- 8:30 – 9:10 *Y. Matsumoto* – A New Approach to the Investigation of Photocatalysis on Atomically Designed Oxide Surfaces and Interfaces  
 9:10 – 9:30 *M. Ikeda* - Scanning Probe Study of Dye-sensitized  $TiO_2(110)$  Surfaces  
 9:30 – 9:50 *I. Lyubinetsky* - Trimethyl Acetate Acid Adsorption Configuration and Photodecomposition on  $TiO_2(110)$   
 9:50 – 10:20 coffee break

**Oral Session 14 Water at Oxide Surfaces** (P. Varga)

- 10:20 – 11:00 *K. Rosso* - Reductive Transformation of Iron Oxides: Coupled Solution and Solid-State Pathways  
 11:00 – 11:20 *S. C. Petito* - Surface Structure and Reactivity of Hydrated Magnetite (111) Under Environmentally Relevant Conditions  
 11:20 – 11:40 *H. Bluhm* - The Interaction of  $H_2O$  and  $NO_2$  with Thin  $MgO(100)$  Films Grown on  $Ag(100)$  as Studied with Ambient Pressure Photoemission Spectroscopy  
 11:40 – 12:00 *P.F. Lyman* - Structure and Lateral Water Ordering at Reconstructed  $MgO(111)$  Surfaces  
 12:00 – 12:15 Closing remarks – announcement of venue for IWOX VI (2009)  
 12:30 – 1:30 Lunch

**Poster Session I – Oxide Surface Structure, Electronic Properties, Photoresponse, Defect Structures, Reactivities, and the Student Poster Competition**

(Monday 8 -10PM + all day Tuesday)

- P1 - *E.I. Altman* - Effect of Ferroelectric Poling Direction on the Structure and Reactivity of LiNbO<sub>3</sub> (0001)
- P2 – *K.M. Beck* - Excitation of Surface Excitons in Magnesium Oxide and Calcium Oxide Nanostructures
- P3 - *S. E. Chamberlin* - DLD-LEED: Low Energy Electron Diffraction Using an Electronic Delay-Line Detector System\*
- P4 - *J.A. Farmer* - Energetics of Calcium and Lithium Adsorption on MgO(100) and its Surface Defects\*
- P5 - *F. Finnochi* - Water Adsorption on Defective Sites at MgO Surfaces: Simulations and Experiments
- P6 - *S. Gritschneider* - Surface Chemistry of CeO<sub>2</sub>(111) Revealed by Dynamic Force Microscopy
- P7 - *S. Gritschneider* - Strong Adhesion of Water to CeO<sub>2</sub>(111)
- P8 – *H. Grönbeck* - NO<sub>2</sub> Charging on Metal Supported Alkaline-earth Metal Oxides
- P9 – *W. Hess* - Mechanisms of Photoinduced Desorption of MgO and CaO Nano-particles
- P10 – *S. Hong* - Reactivity of NO on Stoichiometric RuO<sub>2</sub>(110) : an *ab initio* Study
- P11 – *M. Ikeda* - Scanning Probe Study of Dye-sensitized TiO<sub>2</sub>(110) Surfaces\*
- P12 – *E.S. Ilton* - Beam Induced Reduction of U(VI)-Oxyhydroxide During X-ray Photoelectron Spectroscopy: the Role of the Intermediate Pentavalent Species U(V)
- P13 – *P.A. Jacobson* - Adsorption of Catechol on TiO<sub>2</sub> Surfaces\*
- P14 - *H.T. Johnson-Steigleman* - Dewetting Behavior of Co/MgO(111)\*
- P15 - *D. Le* - CO Oxidation on the Cu<sub>2</sub>O(100) Surface from First Principles\*
- P16 - *J. Matthiesen* - Dynamics of Water Dimers on TiO<sub>2</sub>(110)
- P17 – *K.P. McKenna* – Exciting MgO Nanocrystals

- P18 - *K. Miyashita* - Charge Transfer Between TiO<sub>2</sub> Film and Nanometer-scale Si Overlayer Leading to Improved Photocatalytic Activity\*
- P19 – *H. Onishi* - Low-Frequency Vibrations at TiO<sub>2</sub>(110) Surface Observed with Fourth-Order Raman Scattering
- P20 – *N.G. Petrik* - Electron Stimulated Reactions in Thin Water Films Adsorbed on TiO<sub>2</sub>(110)
- P21 - *S. Shaikhutdinov* - Morphology and Defect Structure of the Ceria Films.
- P22 – *S. Thevuthasan* - Carbon Doping in TiO<sub>2</sub> Using Ion Implantation for Photocatalysis Applications
- P23 - *T. Trevethan* - Simulations of Controlled Single Atom Manipulation on Insulating Surfaces
- P24 - *S. Torbrügge* - Evidence for Subsurface Oxygen Vacancy Arrays on Reduced CeO<sub>2</sub>(111)\*
- P25 – *M.B. Watkins* - Defect chemistry on Ceria (111) Surfaces
- P26 – *Y. Wang* - The Interaction of CO<sub>2</sub> with ZnO Surfaces: Results from a Multi-technique Investigation

\*Competing for Student Poster Prize

**Poster Session II – Oxides on Metals and Metals on Oxides**  
(Wednesday 8-10PM + all day Thursday)

- P1 – *C. Barth* - The Atomic Structure of a Thin Al<sub>2</sub>O<sub>3</sub> Film Grown on Ni<sub>3</sub>Al(111) Revealed by Dynamic Scanning Force Microscopy
- P2 - *C. Barth* - Imaging Nanoclusters in the *Constant Height Mode* of the Dynamic Scanning Force Microscope
- P3 – *M.S. Chen* – Interaction of Metals with Reduced Titania
- P4 - *W.-J. Chun* - Atomically-Dispersed Cu Species on a TiO<sub>2</sub>(110) Surface Premodified with an Organic Compound
- P5 - *M. Delheusy* - In-situ X-ray Study of the Oxide Layer Dissolution on Nb(110) Upon Mild Thermal Treatments
- P6 – *S. Guimond* - Preparation and characterization of Ordered V<sub>2</sub>O<sub>5</sub> and MoO<sub>3</sub> Thin Films on Au(111)

- P7 – *K. Katsiev* - Reactive Metals on the SnO<sub>2</sub> (101) Surface
- P8 - *K. Mašek* - Structural and Spectroscopic Study of Metal/Tungsten Oxide System Prepared on W(110) Single Crystal Surface
- P9 - *K. P. McKenna* - Temperature Dependence of Transient Low Coordinated Sites on Au Nanocrystallites Supported on the MgO(100) Surface
- P10 - *Erie H. Morales* - A Comparative Study of In<sub>2</sub>O<sub>3</sub> and Sn-doped In<sub>2</sub>O<sub>3</sub> Thin Films in (100), (110) and (111) Orientations
- P11 - *D.R. Mullins* - Comparison of the Activity and Morphology of Rh, Pd and Pt Nanoparticles Supported on Ceria Thin Films
- P12 - *N. Nilius* - Influence of Metal-Oxide Interactions on Properties of thin Oxide Films: FeO / Pt(111)
- P13 - *R. Shao* - Structure and Properties of MBE-grown Epitaxial Anatase Films with Rutile Nanocrystalline Inclusions
- P14 - *P. Varga* - Structure of the Antiphase Domain Boundaries in the Ordered Alumina Film on NiAl(110)
- P15 - *R. R. Wixom* - Revisiting the Mechanism of Ionic-Oxide Film Growth on Metals