COST Redox *WG3 Meeting 2014*

2nd Workshop of ***Workgroup 3 (Reactivity)***
CMST COST Action CM1104

Reducible oxide chemistry, structure and functions

May 8-9, 2014
Prague, Czech Republic

Meeting Programme

organized by
Surface Science Group
Department of Surface and Plasma Science
Charles University in Prague

Workshop Programme

Thursday, May 8

9:00-9:10	**Opening**
9:10-9:40	Ordered Phases of Reduced Ceria as Epitaxial Films on Cu(111) *Josef Mysliveček*
9:40-10:10	Progress in modelling of ionic metal species in CeO_2-based catalytic nanomaterials *Konstantin M. Neyman*
10:10-10:40	Hydrogen activation on ceria-supported Pt-Sn nanoalloy particles *Yaroslava Lykhach*
10:40-11:10	**Coffee Break**
11:10-11:40	Relative stability of mononuclear platinum species supported on nanoparticulate ceria and adsorption of CO on them *Hristiyan A. Aleksandrov*
11:40-12:10	Producing CO from CO_2 by redox cycling using doped cerias *N. Raveendran Shiju*
12:10-12:40	Pd@CeO_2 core-shell based catalysts for methane oxidation: Effect of water *Matteo Monai*
12:40-14:30	**Lunch**
14:30-15:15	Fundamental Studies on Model Oxide Catalysts: From UHV to *in-situ* conditions *Dario J. Stacchiola*
15:15-15:45	Substrate effects on Pt nanoparticles. Electronic and structural differences induced by CeO_2(111) and MgO(100) on ~1nm Pt clusters. *Sergey M. Kozlov*
15:45-16:00	**Break**
16:00-19:00	**Poster session** **& Refreshment**

Friday, May 9

9:00-9:30	Effects of Al_2O_3 doping by CeO_2 or MgO on the structural, redox and catalytic properties of Ni catalysts for dry reforming of methane *Leonarda F. Liotta*
9:30-10:00	Morphology, structural defects and oxygen vacancies in $Ce_{1-x}Zr_xO_{2-\delta}$ mixed oxides. Composition dependence, effect of gas atmosphere and preparation methods probed by *in situ* Raman spectroscopy. *Soghomon Boghosian*
10:00-10:30	Model studies of Ni(Pd)-ZrO_2-Pt_3(Pd_3)Zr solid oxide fuel cell anodes *Günther Rupprechter*
10:30-11:00	**Coffee Break**
11:00-11:30	Odd small Cu clusters on ZnO become positive - but even don't! *Matti Hellström*
11:30-12:00	Reactivity of ultra-thin ZnO films supported by Ag(111), Cu(111) and Pt(111) *Shamil Shaikhutdinov*
12:00-12:30	Cobalt Oxide Model Catalyst as Alternative to Noble Metal Catalysts *Christoph Rameshan*
12:30-12:45	**Closing Remarks**
13:00-	**Lunch**

ORAL PRESENTATIONS

THURSDAY

Ordered Phases of Reduced Ceria as Epitaxial Films on Cu(111)

*Tomáš Duchoň, Filip Dvořák, Marie Aulická, Vitalii Stetsovych, Mykhailo Vorokhta, Daniel Mazur, Kateřina Veltruská, Tomáš Skála, **Josef Myslivеček**, Iva Matolínová, and Vladimír Matolín*

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Progress in modelling of ionic metal species in CeO_2-based catalytic nanomaterials

***Konstantin M. Neyman**,[1,2] Albert Bruix,[1] Alberto Figueroba,[1] Francesc Illas,[1] Jörg Libuda,[3] Vladimír Matolín[4]*

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Hydrogen activation on ceria-supported Pt-Sn nanoalloy particles

***Y. Lykhach**,[1] A. Neitzel,[1] T. Skála,[2] N. Tsud,[2] V. Johánek,[2] M. Vorokhta,[2] K. C. Prince,[3] V. Matolín,[2] J. Libuda,[1,4]*

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Relative stability of mononuclear platinum species supported on nanoparticulate ceria and adsorption of CO on them

***Hristiyan A. Aleksandrov**,[1,2] Konstantin M. Neyman,[2,3] Georgi N. Vayssilov*[*,1]*

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Producing CO from CO_2 by redox cycling using doped cerias

*Enrique V. Ramos-Fernandez, **N. Raveendran Shiju**, Gadi Rothenberg*

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THURSDAY (continued)

Pd@CeO_2 core-shell based catalysts for methane oxidation: Effect of water

M. Monai,[1] *T. Montini,*[1] *T. Duchoň,*[2] *N. Tsud,*[2] *E. Fonda,*[3] *C. Chen,*[4] *R.J. Gorte,*[4] *K. Prince,*[5,6] *V. Matolín,*[2] *P. Fornasiero*[1]

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Fundamental Studies on Model Oxide Catalysts: From UHV to *in-situ* conditions

INVITED

Dario J. Stacchiola

Department of Chemistry, Brookhaven National Laboratory, Upton, NY 11973

Substrate effects on Pt nanoparticles. Electronic and structural differences induced by CeO_2(111) and MgO(100) on ~1nm Pt clusters.

Sergey M. Kozlov,[1] *Konstantin M. Neyman,*[1,2] *Stefano Fabris*[3]

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Effects of Al_2O_3 doping by CeO_2 or MgO on the structural, redox and catalytic properties of Ni catalysts for dry reforming of methane

*H. Wu,[1,2] **L. F. Liotta**,[1] G. Pantaleo,[1] V. La Parola,[1] F. Puleo,[1] Xavier Collard,[3] Carmela Aprile,[3] A. M. Venezia[1]*

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[3] Department of Chemistry, University of Namur (UNAMUR), 61 rue de Bruxelles B-5000 Namur, Belgium.

Morphology, structural defects and oxygen vacancies in $Ce_{1-x}Zr_xO_{2-\delta}$ mixed oxides. Composition dependence, effect of gas atmosphere and preparation methods probed by *in situ* Raman spectroscopy.

*Antonios Tribalis and **Soghomon Boghosian***

Department of Chemical Engineering, University of Patras and FORTH/ICE-HT, Patras, Greece

Model studies of Ni(Pd)-ZrO_2-Pt_3(Pd_3)Zr solid oxide fuel cell anodes

*Hao Li, Jake (Joong-Il) Choi,[2] Wernfried Mayr-Schmölzer, Christian Weilach,[1] Christoph Rameshan,[1] Florian Mittendorfer,[2,3] Josef Redinger,[2,3] Michael Schmid[2] and **Günther Rupprechter**[1]*

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2 Institute of Applied Physics, Vienna University of Technology, 1040 Vienna, Austria
3 Center for Computational Materials Science, Vienna Univ. of Techn., 1040 Vienna, Austria

Odd small Cu clusters on ZnO become positive - but even don't!

***Matti Hellström**, Daniel Spangberg, Kersti Hermansson, and Peter Broqvist*

Department of Chemistry - Angstrom Laboratory, Uppsala University, Uppsala, Sweden

Reactivity of ultra-thin ZnO films supported by Ag(111), Cu(111) and Pt(111)

*Q. Pan, B.H. Liu, **S. Shaikhutdinov**, H.-J. Freund*

Chemical Physics Department, Fritz Haber Institute, Faradayweg 4-6, Berlin 14195

Cobalt Oxide Model Catalyst as Alternative to Noble Metal Catalysts

***Christoph Rameshan**, Andrey Bukhtiyarov, Kresimir Anic, Hao Li, Günther Rupprechter*

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POSTER PRESENTATIONS

Size and structure effects controlling the stability of the liquid organic hydrogen carrier dodecahydro-*N*-ethylcarbazole during dehydrogenation over oxide-supported Pt model catalysts

Max Amende, *Christoph Gleichweit, Stefan Schernich, Oliver Höfert, Michael P. A. Lorenz, Wei Zhao, Marcus Koch, Christian Papp, Peter Wasserscheid, Hans-Peter Steinrück, Jörg Libuda*

Friedrich-Alexander-Universität Erlangen-Nürnberg

Synthesis and characterization of mono- and multi-elements (Nb,Sn,Ru)-SBA-12 mesoporous materials

Agnieszka ***Feliczak-Guzik***, *Izabela Nowak*

Adam Mickiewicz University in Poznan, Faculty of Chemistry, Poznan, Poland

In-situ IR Spectroscopy on Modified Pt Catalysts for Steam Reforming and Fuel Cells

A. Kaftan,[1] *O. Brummel,*[1] *F. Faisal,*[1] *T. Bauer,*[1] *F. Kollhoff,*[2] *M. Kusche,*[2] *H. Niedermeyer,*[2] *P. Wasserscheid,*[2] *I. Khalakhan,*[3] *V. Matolín,*[3] *M. Laurin,*[1] *J. Libuda*[1]

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IRAS Study of CO Adsortion and Coadsorption on Cobalt Oxide Model Catalysts

Arafat Toghan,[1] *Sascha Mehl,*[1] *Balázs László,*[1,2] *Jörg Libuda*[1]

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The interaction of H_2 with Pt-Sn particles on a tin-ceria mixed oxide film

Armin Neitzel,[1] *Yaroslava Lykhach,*[1] *Tomáš Skála,*[2] *Nataliya Tsud,*[2] *Viktor Johánek,*[2] *Mykhailo Vorokhta,*[2] *Kevin C. Prince,*[3,4] *Vladimír Matolín,*[2] *Jörg Libuda*[1,5]

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Combined XPS and DRIFTS examination of the reduction under CO of Cu/CeO_2 CO-PROX catalysts

Manuel Monte,[1] *Guillermo Munuera,*[2] *José C. Conesa,*[1] ***Arturo Martínez-Arias***[1,*]

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Gold catalysts on Pr-modified ceria for pure hydrogen production via WGS reaction: effect of gold dispersion and redox properties depending on the preparation method of mixed supports

L. Ilieva Gencheva,[1] *T. Tabakova,*[1] *P. Petrova,*[1] *I. Ivanov,*[1] *G. Munteanu,*[2] *M. Boutonnet,*[3] *J.W. Sobczac,*[4] *W. Lisowski,*[4] *Z. Kaszkur,*[4] *G. Pantaleo,*[5] *A.M. Venezia*[5]

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CO on clean and oxidized Pd(111): A combined photoelectron, vibrational spectroscopy and DFT study

Maxime Van den Bossche,[1] *Natalia Martin,*[2] *Edvin Lundgren,*[2] *Feng Zhang,*[3] *Li Tao,*[3] *JasonWeaver,*[3] *Henrik Gronbeck*[1]

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Interactions between the room-temperature ionic liquid [C_2C_1Im][OTf] and Pd(111), well-ordered Al_2O_3, and supported Pd model catalysts studied by infrared spectroscopy

Stefan Schernich, *Dmytro Kostyshyn, Valentin Wagner, Nicola Taccardi, Mathias Laurin, Peter Wasserscheid, Jörg Libuda*

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In-situ IRAS Studies of Disubstituted Benzenes on MgO(100)/Ag(100)

S. Mohr,[1] *T. Xu,*[1] *T. Döpper,*[2] *A. Görling,*[2] *M. Laurin,*[1] *J. Libuda*[1]

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Applicability of Fe-modified ceria as support of mono and bimetallic Au-Pd catalysts for complete benzene oxidation

T. Tabakova,[1] *L. Ilieva,*[1] *P. Petrova,*[1] *A.M. Venezia,*[2] *G. Avdeev*[3]

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Synthesis, characterization and catalytic activity of mesoporous silica materials with SBA-15-like structure modified with amino groups

***Agata Wawrzyńczak**, Magdalena Górzyńska and Izabela Nowak**

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Magnetron sputtered Pt-CeO_2 thin film catalyst for PEM fuel cell applications

***M. Vorokhta**,[1] I. Khalakhan,[1] A. Rednyk,[1] R. Fiala,[1] M. Václavů,[1] I. Matolínová,[1] H. Yoshikava,[2] V. Matolín[1]*

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Bonding of Adenine to cerium oxide

***Sofiia Bercha**[1], Nataliya Tsud[1], Klára Ševčíková[1], Robert G. Acres[2], Kevin C. Prince[2], Vladimír Matolín[1]*

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How the interaction between Rh and CeO_x influences CO oxidation

***Klára Ševčíková**,[1] Tatiana Zahoranová,[1] Nataliya Tsud,[1] Tomáš Skála,[1] Vladimír Matolín,[1] Yaroslava Lykhach,[2] and Václav Nehasil[1]*

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