

# Workshop Programme

## Wednesday, September 26

<b>14:00-14:10</b>	<b>Opening</b>
<b>14:10-14:35</b>	Environmental effects and reactivity of iron oxide films on Pt(111) <i>Livia Giordano</i>
<b>14:35-15:00</b>	Understanding the high reducibility of gallium(III)-doped ceria <i>Monica Calatayud</i>
<b>15:00-15:20</b>	Insight into the adsorption of water on the clean CeO <sub>2</sub> (111) surface with van der Waals and hybrid density functionals <i>Delia Fernández-Torre</i>
<b>15:20-15:40</b>	Polarity in low dimensions: MgO nano-islands on Au(111) <i>Jacek Goniakowski</i>
<b>15:40-16:00</b>	Simulated Photoemission Spectra of Hydroxylated MgO(100) at Elevated Temperatures <i>Lauro Oliver Paz-Borbón</i>
<b>16:00-16:30</b>	<b>Coffee Break</b>
<b>16:30-16:55</b>	DFT and HR-STEM investigations into morphology and electronic structure of Co <sub>3</sub> O <sub>4</sub> redox nanooxide <i>Filip Zasada</i>
<b>16:55-17:20</b>	A novel 2-D ternary Cu-tungstate phase on Cu(110)2x1-O surface oxide <i>Falko P. Netzer</i>
<b>17:20-17:40</b>	Design of novel WO <sub>3</sub> -based materials with tailored optical, photo-redox or catalytic properties <i>Cristiana Di Valentin</i>
<b>17:40-18:00</b>	Packing Defects into Ordered Structures <i>Henrik H. Kristoffersen</i>
<b>18:00-18:20</b>	Ordered Array of Single Au Adatoms on Fe <sub>3</sub> O <sub>4</sub> (001) with Remarkable Thermal Stability <i>Zbynek Novotny</i>
<b>18:20-18:40</b>	Free energy calculation for the H abstraction from propane by V <sub>2</sub> O <sub>5</sub> /SiO <sub>2</sub> : Molecular dynamics compared to harmonic approximation <i>Witold Piskorz</i>
<b>20:00-23:00</b>	<b>Dinner</b>

## Thursday, September 27

<b>8:30-8:55</b>	Unified Picture of the Excess Electron Distribution at the TiO <sub>2</sub> (110) Surface <i>Jacques Jupille</i>
<b>8:55-9:20</b>	(Sub)surface oxygen vacancies on TiO <sub>2</sub> anatase (101) and O <sub>2</sub> adsorption <i>Martin Setvín</i>
<b>9:20-9:40</b>	Exploring the electronic structure and optical excitations of F-doped TiO <sub>2</sub> : Relevance to Photocatalysis <i>Francesc Illas</i>
<b>9:40-10:00</b>	Domain walls of CO adlayers on Pd nanoparticles <i>Geoff Thornton</i>
<b>10:00-10:20</b>	Mechanism of Surface Reactions: Insights from First Principles Calculations <i>Javier Fdez. Sanz</i>
<b>10:20-11:00</b>	<b>Coffee Break</b>
<b>11:00-11:25</b>	(VO <sub>n</sub> ) <sub>m</sub> (n = 1, 2; m = 1 – 3) submonolayers supported on the CeO <sub>2</sub> (111) surface: Insights into structure and reactivity of a complex catalytic system from density functional theory <i>Joachim Paier</i>
<b>11:25-11:50</b>	In-situ nanoscale redox chemistry of cerium oxide islands on Ru(0001) <i>Jan Ingo Flege</i>
<b>11:50-12:10</b>	Recent progress in density functional studies of ceria-based nanostructures <i>Konstantin M. Neyman</i>
<b>12:10-12:30</b>	DRIFTS and XPS <i>operando</i> studies of an inverse CeO <sub>2</sub> /CuO water-gas shift catalyst <i>Arturo Martínez-Arias</i>
<b>12:30-12:50</b>	Thin film cerium oxide based catalysts for fuel cell application <i>Vladimír Matolín</i>
<b>12:50-13:50</b>	<b>Lunch</b>

<b>13:50-14:15</b>	Decomposition pathways of carboxylic acid on Pt/ceria model catalysts <i>Yaroslava Lykhach</i>
<b>14:15-14:35</b>	DFT study of Zn-Ti oxide photocatalysts <i>José C. Conesa</i>
<b>14:35-14:55</b>	Atomistic structure of cobalt-oxide/phosphate nanoparticles for catalytic water oxidation <i>Stefano Fabris</i>
<b>14:55-15:15</b>	Influence of carbon-carbon bond order and silver loading on the oxidative function of silver-alumina catalysts in absence and presence of NO <i>Hanna Härelind</i>
<b>15:15-15:35</b>	The application of high-resolution IR spectroscopy and isotope labeling for detailed investigation of TiO <sub>2</sub> /gas interface reactions. <i>Svatopluk Civiš</i>
<b>15:35-18:00</b>	<b>Coffee Break &amp; Poster Session</b>
<b>16:30-20:00</b>	<b>MC Meeting</b>

## Friday , September 28

<b>8:30-8:55</b>	Imidazolium-based ionic liquids interacting with ordered cerium dioxide surfaces: a synchrotron-radiation photoelectron spectroscopy study <i>Mathias Laurin</i>
<b>8:55-9:20</b>	Tuning metal-support interactions in reducible Pd@CeO <sub>2</sub> core shell based catalysts <i>Paolo Fornasiero</i>
<b>9:20-9:40</b>	Active sites for methane dissociation over metallic and oxidized palladium <i>Henrik Grönbeck</i>
<b>9:40-10:00</b>	Potential method for detecting oxygen vacancies in oxides <i>Filip Tuomisto</i>
<b>10:00-10:20</b>	Facilitated lattice oxygen depletion in consolidated TiO <sub>2</sub> nanocrystal powders: a spectroscopic O <sub>2</sub> adsorption study <i>Oliver Diwald</i>
<b>10:20-11:20</b>	<b>Coffee Break &amp; Lab Tour</b>
<b>11:20-11:45</b>	First principles calculations of formation and migration of oxygen vacancies in La <sub>1-x</sub> Sr <sub>x</sub> Co <sub>1-y</sub> Fe <sub>y</sub> O <sub>3-δ</sub> perovskites <i>Yuri A. Mastrikov</i>
<b>11:45-12:05</b>	Solar Cells with Overall Water Splitting Using Oligoaniline-Crosslinked [Ru(bpy) <sub>2</sub> (bpyCONHArNH <sub>2</sub> )] <sup>+2</sup> Dye/Iridium Oxide Nanoparticle Arrays On Three-Dimensionally Ordered Macroporous Gold-Nanoparticle Doped Titanium Dioxide (3-DMGN-TiO <sub>2</sub> ) Photonic Crystals Modified Electrodes <i>Huseyin Bekir Yildiz</i>
<b>12:05-12:25</b>	Electronic processes at metal/oxide interfaces <i>Alexander L. Shluger</i>
<b>12:25-12:45</b>	Impact of oxygen scavenging on electronic properties of thin HfO <sub>2</sub> layers <i>Valery V. Afanas'ev</i>
<b>12:45-12:55</b>	<b>Closing Remarks</b>