

## O 72: Competition for the Gerhard Ertl Young Investigator Award

Time: Thursday 10:30–13:00

Location: PHY C 213

O 72.1 Thu 10:30 PHY C 213

**Fundamental aspects of germanium surface passivation by gas phase oxidation and liquid phase sulfidation** —

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To fully explore the potential germanium may offer for device application the effective and reliable passivation of defect states is essential (A. Dimoulas et al. 2007). In this contribution we will present two promising passivation schemes for Ge(100) surfaces: The in situ oxidation and ex situ sulfidation. By applying complementary analysis techniques we were able to investigate -at the atomic level- the adsorption mechanisms and surface properties of these O/Ge(100) and S/Ge(100) systems. We will show that both treatments result in discontinuous (sub-monolayer) self-limiting adsorbate layers. The adsorption geometry is comparable between both passivation schemes, and similarities are observed in view of passivation of intrinsic unoccupied defect states in the Ge band gap. The overall quality of the passivation layer appears to be limited by intrinsic and extrinsic constraints.

O 72.2 Thu 11:00 PHY C 213

**Unraveling Elementary Electron Scattering Processes Using Ultrafast Photoemission** — •PATRICK KIRCHMANN — Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Menlo Park CA, USA

Femtosecond time- and angle resolved photoemission spectroscopy is becoming a powerful tool for resolving elementary electron scattering processes directly in the time domain. Measurement of the transient single-particle function grants simultaneous access to single- and many-body information with energy and momentum resolution only few methods can deliver. In this contribution, we highlight these exciting capabilities by discussing (i) quasi-particle lifetimes due to electron-electron scattering in quasi-two-dimensional Pb quantum wells and their relation to Fermi liquid theory [1], (ii) optical excitation pathways and phonon-mediated surface-to-bulk scattering in the topological insulator compound Bi<sub>2</sub>Se<sub>3</sub> [2], and (iii) the collective response of the amplitude mode in the charge density wave compound TbTe<sub>3</sub> [3]. These results provide qualitatively new insights into the dynamics of optically excited electrons and the collective response of emergent phases in quantum materials.

[1] Nature Physics 6, 782 (2010)

[2] PRL 108, 117403 (2012); PRL 111, 136802 (2013)

[3] Science 321, 1649 (2008)

O 72.3 Thu 11:30 PHY C 213

**Digging up the band structure of buried layers** — •JILL MIWA<sup>1</sup>, PHILIP HOFMANN<sup>1</sup>, OLIVER WARSCHKOW<sup>2</sup>, DAMIEN CARTER<sup>3</sup>, NIGEL MARKS<sup>3</sup>, MICHELLE SIMMONS<sup>4</sup>, and JUSTIN WELLS<sup>5</sup> — <sup>1</sup>Aarhus University, Denmark — <sup>2</sup>University of Sydney, Australia — <sup>3</sup>Curtin University, Australia — <sup>4</sup>UNSW, Australia — <sup>5</sup>NTNU, Norway

Atomically precise dopant placement opens up an exciting new arena for exploring complex valley physics in novel materials and quantum electronic devices. Atomic scale devices derived from phosphorus  $\delta$ -layers in silicon have been recently demonstrated, including a single-atom transistor. A  $\delta$ -layer is formed several nanometers beneath the surface of silicon because of a one-atom-thick plane of phosphorus dopants which are placed there. The local but strong doping leads to confined 2D electron states, separated by an energy referred to as

valley splitting. The magnitude of the valley splitting has implications for critical device properties. Hitherto only indirect information on the electronic structure of the 2D states and valley splitting was available and a reliance on calculations has been necessary. We directly measure the band structure of a buried  $\delta$ -layer using ARPES. Although the  $\delta$ -layer is deeply buried, relative to the photoelectron mean free path, photoemission is still possible at very low kinetic energies, or when a resonant enhancement is invoked. By engineering a favourable surface Umklapp process, we can resolve the  $\delta$ -layer states and measure a valley splitting of 132meV, which falls centrally within reported calculated values. Electronic properties, such as valley splitting, are central in understanding  $\delta$ -layers and their use in atomic-scale devices.

O 72.4 Thu 12:00 PHY C 213

**PdZn and CuZn model catalysts for methanol steam reforming - Structure selectivity correlations obtained by in-situ surface spectroscopy and catalytic testing** —

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Methanol Steam Reforming is a promising reaction for the renewable Energy Scenario. The reaction must be carried out with a high selectivity, avoiding the undesired by-product CO, which poisons the fuel-cell electrocatalyst. Apart from advanced copper based catalysts, reduced states of Pd/ZnO or Pd/Ga<sub>2</sub>O<sub>3</sub> have been identified as promising candidates. This work was focused on PdZn and CuZn model catalysts and their activity and selectivity. Exact correlation between their catalyst structure and the catalytic performance were shown through synchrotron based in-situ ambient pressure XPS measurements. It could be shown that only a sufficient thick PdZn intermetallic phase with a corrugated surface (Zn out, Pd in) is an excellent catalyst.

O 72.5 Thu 12:30 PHY C 213

**Cost-Effective Catalysis on Early Transition Metal Carbides Surfaces** — •FRANCESC VIÑES — Universitat de Barcelona, Barcelona, Spain

Most of the reactions carried out in the industry are catalyzed on the surface of materials, which oftentimes are late transition metals, given its ideal properties as catalytic active phases. However, coinage and Pt-group metals can be quite expensive mainly due to their scarcity, which led to the utilization of metal nanoparticles supported on oxide supports, thus partially alleviating the economic burden.

Early transition metal carbides have been introduced in the last decade as a low-cost alternative to late transition metals. Beyond the comparable electric and thermic conductivities, they present physical robustness, and, eventually, a catalytic activity comparable, or even superior, to late transition metals. Here we show, by ab initio density functional calculations combining experimental results, how different surfaces of such carbides are adequate catalytic active phases for a variety of reactions, including the water-gas-shift reaction and the dissociation of small molecules, such as oxygen, hydrogen, and even carbon dioxide. Moreover, these carbides result to be excellent supports for late transition metal clusters, playing also the role of promoters; the carbide surface is able to polarize the late transition metal electron density, leading to an enhanced catalytic activity, as shown to be critical in the decomposition of sulfur-containing species such as sulphur dioxide and thiophene. Future fields of applications are envisaged.