

## MM 34: SYM Hydrogen in Materials: New Developments II

Time: Thursday 11:40–12:50

Location: H 1058

**Invited Talk** MM 34.1 Thu 11:40 H 1058  
**The Interaction of Hydrogen with Metal Surfaces: Molecular Precursors, Chemisorbed Atoms and Subsurface States** —  
 •KLAUS CHRISTMANN — Institut für Chemie und Biochemie der FU Berlin, 14195 Berlin

In this contribution, the scenario of hydrogen interaction with (single-crystalline) metal surfaces will be surveyed including physisorbed and chemisorbed molecular hydrogen, dissociative (atomic) hydrogen adsorption, and subsurface H state population, whereby both energetic and kinetic phenomena will be considered. Special attention is devoted to H-induced structural changes of the surface region of the exposed crystal (relaxation and reconstruction), on subsurface state population and especially on molecularly chemisorbed hydrogen. Relatively strongly bound adsorbed hydrogen molecules may play an important role as a precursor during H uptake and storage processes, and recent results obtained for H and H<sub>2</sub> interacting with the (210) surfaces of the fcc metals Ni, Pd and Rh will be presented.

MM 34.2 Thu 12:10 H 1058  
**Thermodynamic aspects of the hydrogen absorption in nano-metallic clusters** — •MOHAMMED SULEIMAN, REINER KIRCHHEIM, and ASTRID PUNDT — Institute of Material Physics, University of Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany

Metallic nano-sized clusters (2.0-6.0 nm) have been shown to have distinct differences in their hydrogen uptake characteristics when compared to bulk Pd. These differences are not only due to the different physical properties of the small-size system but they could be affected by the stabiliser and, also, by the cluster structure. In this work the thermodynamic absorption behaviour of hydrogen in nm-sized metal-

lic clusters with different size and different structure will be presented. The phase transition in these samples was monitored by in situ X-ray diffraction and in situ EXAFS measurements during hydrogen loading. The thermodynamic behaviour of hydrogen absorption will be presented using P-c Isotherm, P-d Isotherms and P-R Isotherm. It will be shown that the phase boundaries and the hydrogen uptake ability in these samples depends strongly on the lattice structure which is affected by the type of metallic clusters and the stabilizer used in samples.

MM 34.3 Thu 12:30 H 1058  
**MC-MD simulations of pressure-concentration isotherms for Hydrogen in bulk Palladium and clusters** — •DIANA MARCANO and HELMAR TEICHLER — Institut fuer Materialphysik, Universitaet Goettingen

For nanoscale Pd clusters loaded with H experimental pressure - concentration isotherms resemble those for bulk material, with the main difference of a finite slope instead of the two-phase regime and a narrowing of this region compared to bulk. Regarding this, we here present results from MC-MD studies using for the chemical potential a new calculation scheme, which means an extension of Widom's particle insertion method. The simulations rely on the Tomanek model with improved H-Pd coupling for properly taking care of lattice deformations and modified H-H interaction including first and second neighbour interactions. For bulk material, the asymmetric two-phase regime is obtained, extending up to 62 % H. The results for a 923 Pd atoms cuboctahedral cluster reflect the variation of site energies in the cluster where the shift to lower H concentrations is related to the interplay between first and second neighbour H-H interactions.