

Gegründet im Jahre 1869 von H. Hlasiwetz, J. Loschmidt, J. Petzval und J. Stefan

## **Loschmidt Preis 2003**

der

Chemisch-Physikalischen Gesellschaft

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## Holographic Scattering in Electro-optic Crystals

A detailed experimental study of holographic scattering (HS) in  $LiNbO_3$ : Fe and SNB: Ce crystals, representing local and non-local recording media, respectively, is performed. The characteristics of parasitic holograms (PH) are different in these two types of photorefractives. However, the main features of PH can be explained by a simple phenomenological model based on the Ewald sphere construction. The obtained results enable us to choose read-out conditions for which the effect of HS can be either minimized or exploited to give valuable information about the recording medium. Moreover, the effect of applying electric field and stoichiometry on HS is investigated. In addition, HS is introduced for the first time as a simple and accurate technique for the determination of the activation energy for thermal fixing in photorefractive crystals.

Dr. Robin HIRSCHL

Institut für Materialphysik der Universität Wien Betreuer: O.Univ.Prof. Dr. Jürgen Hafner

## Binary Transition Metal Alloys and Their Surfaces - an Ab Initio Study

Alloys often exhibit physical and chemical properties that are very different from the ones of the individual constituents. Theoretical and technological advances in the last years have extended the applicability of computer simulations from first principles towards even more complex systems. The presented work is devoted to the investigation of binary transition metal alloys, particularly their surfaces, from first principles in the framework of density functional theory. Properties of interest are mainly their chemical reactivity and catalytic properties as compared to the pure-metal surfaces. Starting with clean surfaces, the Pd(111) surface alloyed with submonolayer amounts of vanadium allows to investigate the influence of an "early" transition-metal on a "late" transition metal surface on atomic scales. In a second step the influence of alloying on the adsorption of simple molecules such as CO is described. Eventually we simulated chemical reactions, namely the dissociation of  $H_2$  and the hydrogenation of unsaturated aldehydes, on alloy surfaces. Among the surprising findings is the first identification on an intrinsic molecular precursor in the dissociate absorption of  $H_2$  over a close-packed transition-metal surface.

Die Preisverleihung und die Festvorträge finden am

Montag, dem 26. Jänner 2004, um 10 Uhr c.t.

im Kleinen Hörsaal des Instituts für Experimentalphysik der Universität Wien, 1090 Wien, Strudlhofgasse 4/Boltzmanngasse 5, 2. Stock statt.