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# IAP-SEMINAR

## EINLADUNG

Termin: **Dienstag, 23.11.2010 um 16:00 Uhr**  
Ort: **Technische Universität Wien,  
Institut für Angewandte Physik,  
Seminarraum 134A, Turm B (gelbe Leitfarbe), 5. OG  
1040 Wien, Wiedner Hauptstraße 8-10**

Vortragender: **Dr. Frantisek Máca**  
Institute of Physics ASCR, Prague/CZ

Thema: **Magnetic order in the ultrathin iron film on the Ir(001) surface**

### Kurzfassung

We present detailed ab initio study of structural and magnetic stability of a Fe monolayer on the fcc (001) surface of iridium. The Fe monolayer has a strong tendency to order antiferromagnetically for the true relaxed geometry [1]. The ferromagnetism is stabilized by the increased Fe-Ir layer spacing. The present study centers around the evaluation of pair exchange interactions between Fe atoms in the Fe overlayer as a function of adsorbate coverage which allows for a detailed understanding of the antiferromagnetism of a Fe/Ir(001) overlayer. Our calculations indicate that the nature of the true ground state could be more complex and display a spin spiral like rather than a c(2x2)-antiferromagnetic order.

We compare the influence of two adsorbate species, H and O, on the magnetic ground state. We found that the adsorption of oxygen (contrary to the H) lowers the stability of antiferromagnetic order and prefers ferromagnetic ground state. The scanning tunnelling spectroscopy shows a surface state, its energy position varied with iron coverage. We present how the magnetic order and the iron coverage influence the surface state appearance. A comparison with recent experimental data will be also given.

[1] J. Kudrnovský, F. Máca, I. Turek, and J. Redinger, Phys. Rev. B 80, 064405 (2009).

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*Alle interessierten Kolleginnen und Kollegen sind zu diesem Seminar  
(45 min mit anschließender gemeinsamer Diskussion) herzlich eingeladen.*

*J. Redinger e.h.  
(Seminar-Chairperson)*

*H. Störi e.h.  
(LVA-Leiter)*