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INSTITUT FÜR  
ANGEWANDTE PHYSIK  
Institute of Applied Physics  
vormals/formerly  
Institut für Allgemeine Physik



Wiedner Hauptstraße 8-10/E134, 1040 Wien/Vienna, Austria – Tel: +43 1 58801 13401 / Fax: +43 1 58801 13499 – E-mail: [office@iap.tuwien.ac.at](mailto:office@iap.tuwien.ac.at) / <http://www.iap.tuwien.ac.at>

# IAP-SEMINAR

## ANNOUNCEMENT CHANGE OF DATE

- Date: **Tuesday, 22.11.2016** (primary 8.11.)  
Time: **16:00 s.t.**  
Location: **Technische Universität Wien, Institut für Angewandte Physik, E134**  
yellow tower „B“, 5<sup>th</sup> floor, Sem.R. DB gelb 05 B (room number  
DB05L03), 1040 Wien, Wiedner Hauptstraße 8-10
- Lecturer: **Privatdoz. Dr. Sergii Khmelevskiy**  
TU Wien, IAP, Center for Computational Materials Science
- Subject: **Functional Antiferromagnetic Materials for Spintronics**  
**Applications: Challenge for Ab Initio Computations**
- Abstract: With the discovery of the Giant Magneto Resistance (GMR) effect antiferromagnetic materials became of ultimate importance in modern electronics since they provide a pinning of the ferromagnetic layers. Devices containing these materials are an integral part of almost any modern computer memories. Due to the recent development of laser assisted ultrafast switching of the magnetization in ferri- and antiferromagnets (AFM), new routes for application of spin-orbit coupling effects in spintronics have been opened. The search of new AFM materials for applications, with stringent technological requirements on their properties, became main stream in the developments in magnetic materials science.  
In this talk I will give an overview of the subject and illustrate the major role of first-principles modeling in the AFM material development. I will discuss the discovery of the new high-temperature AFM materials, the development of new routes in spintronics using ab initio modeling, the application of the magnetic force theorem for predicting the Néel temperature and local anisotropies in functional AFM alloys on realistic materials like  $Mn_2Au$ ,  $Ru_2MnX$ ,  $V_3Al$ ,  $Mn_3Ga$ , binaries  $Mn(Ir,Pd,Ni)$  etc. The emergence of ferromagnetic materials in spintronics as an alternative to ferri- and antiferromagnetic materials in connection with laser ultrafast magnetization switching technology will also be discussed. I will show how the ab-initio based methods may be applied for simulation of the magnetization switching process in ferrimagnets and domain walls in classical ferromagnets (hcp Co).

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*All interested colleagues are welcome to this seminar lecture  
(45 minutes presentation followed by discussion).*

*P. Mohn e.h.*  
(Seminar-Chairperson)

*F. Aumayr e.h.*  
(LVA-Leiter)