



Leibniz-Institut  
für Festkörper- und  
Werkstoffforschung  
Dresden

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Einladung zum

# ITF-Seminar

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**Dr. Stefaan Cottenier**

Center for Molecular Modeling (CMM), Ghent University, Belgium

## $\gamma'$ -Fe<sub>4</sub>N: facts, hypotheses and open questions

By reviewing the experimental and theoretical literature on  $\gamma'$ -Fe<sub>4</sub>N, and by a systematic survey of predictions by the LDA, PBE, WC, LDA+U (2x), PBE+U (2x), and B3PW91 exchange-correlation functionals, the structural, magnetic and hyperfine properties of this material as well as their pressure dependencies are interpreted. The hypothesis is put forward that  $\gamma'$ -Fe<sub>4</sub>N as found in nature is exactly at a sharp transition between low-spin and high-spin behaviour. PBE+U (U=0.4 eV) is identified as the most accurate exchange-correlation functional for this material, although it is needed to fix the magnetization at the experimental value to obtain a satisfying description. Remaining disagreement between theory and experiment is pointed out. A recent experimental claim for a giant magnetic moment in  $\gamma'$ -Fe<sub>4</sub>N is discussed, and is not reproduced by our calculations.

This seminar is based on a review article by Eitel L. Peltzer y Blancá, Judith Desimoni, Niels E. Christensen, Heike Emmerich and SC, *Physica Status Solidi B* **246** (2009) 909-928 (<http://dx.doi.org/10.1002/pssb.200844401>).

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**Montag, 21 September, 2009**

**13:00 Uhr**

**D2.E.27**

IFW Dresden  
Helmholtzstraße 20

Einladender: PD Dr. Manuel Richter