MA 5: Invited Talks Pätzold / Gruner

Time: Monday 14:00–15:00 Location: H10

Invited Talk MA 5.1 Mon 14:00 H10

Novel magnetoresistive effect in organic semiconductors — •Ralph Paetzold, Manfred Ruehrig, and Joachim Wecker — Siemens AG, CT MM1, Guenther-Scharowsky-Strasse 1, 91058 Erlangen, Germany

Besides the more classical organic applications like organic PV and organic LEDs organic semiconductors have also been demonstrated to show a significant magnetoresitive effect. In 2004 the first article on the so called OMR (organic magnetoresistive effect) was published by T. Francis et al [1]. Devices that show significant OMR effect are quite similar to standard OLEDs in terms of materials and device architecture. The effect itself can vary with materials and the device architecture used. In this contribution we will give an overview about the general effect and discuss some possible causes. Experimental results will be introduced in order to evaluate the different mechanisms.

Invited Talk MA 5.2 Mon 14:30 H10

Structural and magnetic properties of transition metal nanoparticles from first principles — •Markus Ernst Gruner, Georg Rollmann, Alfred Hucht, and Peter Entel — Dept. of Physics, University of Duisburg-Essen, Campus 47048 Duisburg

Until recently, the simulation of transition metal particles in the nanometer range was only feasible with semi-empirical approaches and classical molecular dynamics simulations. However, the close interrelation of electronic and structural properties often leaves no alternative to a fully quantum mechanical treatment. The evolution of modern supercomputer technology nowadays allows for the simulation of nanometer-sized objects from first principles in the framework of the density functional theory (DFT). A technologically relevant example is the search for ultra-high density magnetic recording media where the decrease of the magnetic grain size competes with the inset of superparamagnetism. Here, FePt nanoparticles are discussed as a promising solution due to their large magnetocrystalline anisotropy in the ordered $L1_0$ phase. However, in experiment also other, less favorable, structures are observed. Therefore, a systematic *ab initio* investigation of the morphologies of FePt particles concerning their energetics and magnetism at sizes relevant for future application appears highly desirable. Within this contribution, we report on DFT calculations of Fe and FePt clusters of up to 561 atoms including full geometric optimization. The calculations were carried out using the Vienna Ab initio Simulation Package (VASP) on up to 2048 processors on the IBM BlueGene/L installation at Forschungszentrum Jülich.