MA 29: Magnetic Semiconductors I

Time: Thursday 15:15–16:45 Location: H22

MA 29.1 Thu 15:15 H22

Defect pairing and magnetism in C or N-doped MgO and ZnO: a density-functional study — •Peter Kratzer[1], Hua Wu[2], Sung Sakong[1], Xin-Gao Gong[3], and Matthias Scheffler[4] — [1]Fakulät für Physik, Universität Duisburg-Essen, D-47048 Duisburg, Germany — [2]II. Physikalisches Institut, Universität zu Köln, D-50937 Köln, Germany — [3]Fudan University, Shanghai, China — [4]Fritz-Haber-Institut der MPG, D-14195 Berlin, Germany

It is demonstrated that C or N doping recently proposed as a way to create magnetism in otherwise nonmagnetic oxide insulators is curtailed by formation of defect pairs. Our density-functional calculations show that N-N pairing in MgO lowers the energy by 0.4 eV, leading to a nonmagnetic state. C-C pairing is even exothermic by more than 3 eV, and the resultant $(C\text{-}C)^{4-}$ molecules with spin=1 couple antiferromagnetically in MgO. However, calculations for C-doped ZnO, when properly treated using the PBE0 hybrid functional, show that the spin-polarized $pp\pi^*$ levels resonate with the host conduction band, which could possibly mediate a long-range ferromagnetic order. Magnetism of open-shell *impurity molecules* is proposed as a possible route to d^0-ferromagnetism in oxide spintronic materials.

MA 29.2 Thu 15:30 H22

Magnetic Effects of Defect Pairs in Zinc Oxide — •Waheed Adeagbo[1], Guntram Fischer[1], Arthur Ernst[2], and Wolfram Hergert[1] — [1]Institute of Physics, MLU Halle-Wittenberg, Von-Seckendorff-Platz 1, 06120 Halle, Germany — [2]Max Planck Institute for Microstructure Physics, Weinberg 2, 06120 Halle, Germany

In order to gain insight into intrinsic and extrinsic d^0-magnetic properties of defectious ZnO we have carried out *ab initio* calculations on various types of defects formed by substitutionally doped atoms, Zn vacancies, and doped atom and vacancy defect pairs. The doped atoms include N and H which substitute either O or Zn lattice sites. The largest magnetic moment is induced when a Zn vacancy pair is created. Our results also show that some defects that are magnetic when isolated can become non-magnetic when being near other defects. We also investigate the magnetic interaction of different defect pairs. The results of total energy calculations show in all cases the stability of ferromagnetic configurations when compared to the antiferromagnetic counterparts. This characteristic is the strongest for the Zn-Zn vacancy.

MA 29.3 Thu 15:45 H22

Ab-initio **study of zinc oxide surfaces and interfaces in presence of cobalt clusters** — •Sanjeev K. Nayak, Heike C. Herper, and Peter Entel — University of Duisburg-Essen, 47057 Duisburg, Germany

The magnetic properties of Co doped ZnO are controversially discussed in both theory and experiment. Cationic substitution of Co in ZnO bulk shows ferromagnetic properties only if the concentration of Co exceeds the percolation threshold. The Curie temperature is always below room temperature (RT). In order to enhance the Curie temperature above RT, which is necessary for spintronics applications, lattice defects and the ZnO surfaces play an important role. In addition, not only doped bulk ZnO is of interest but also ZnO nanoclusters with embedded Co clusters.

In this contribution we present results of migration of single doped Co atom and of small Co clusters from the center of ZnO to the surface. This self-purification is of primary interest and hindering successful doping of ZnO nanomaterials [1,2]. We investigate various ZnO surfaces and their structural and magnetic properties in presence of Co impurities. In particular clustering effects over the ZnO surfaces will be discussed.

[1] M. Opel et al., Eur. Phys. J. B, **63**, 437 (2008), [2] G. M. Dalpian et al., Phys. Rev. Lett. **96**, 226802 (2006)

MA 29.4 Thu 16:00 H22

Thermodynamical limits of diluted magnetic semiconductors — •Danilo Bürger, Michael Seeger, Shengqiang Zhou, Manfred Helm, and Heidemarie Schmidt — Forschungszentrum Dresden-Rossendorf e.V., Bautzner Landstraße 400, 01328 Dresden

The incorporation of transition metals dopants in semiconductors over their solubility limit is the main challenge for the fabrication of diluted ferromagnetic semiconductors. Dietl et al. [1] calculated the Curie temperatures for various semiconductors doped with 5 at% Mn. A lot of experimental effort was focused on the fabrication of diluted magnetic semiconductors. Unfortunately, such metastable alloys try to reach their thermodynamical equilibrium by the diffusion of the incorporated dopants. The equilibrium state at room temperature for semiconductors with a low solubility of magnetic dopant atoms is characterized by unwanted secondary phases. We present the results from combined random walk simulations and heatflow calculations and explain the successful fabrication of GaAs:Mn and the impossibility to produce diluted Si:Mn. The clustering process is simulated under the assumption that neighbouring magnetic atoms stick together. This is a general approach for the growth of clusters in supersaturated materials [2]. With the knowledge of the diffusion coefficient our modelling can be used to predict the thermodynamical limit at room temperature and the producibility by pulsed laser annealing of diluted magnetic semiconductors. [1] T. Dietl, H. Ohno, F. Matsukura, J. Cibert, and D. Ferrand, Science **287**, 1019 (2000) [2] P. Meakin, Fractals, scaling and growth far from equilibrium (Cambridge University Press, 1998)

MA 29.5 Thu 16:15 H22

Secondary phase formation in (Zn,Mn)O and its influence on the magnetic properties — •Gillian Kiliani[1], Mikhail Fonin[1], Ulrich Rüdiger[1], Reinhard Schneider[2], Dimitri Litvinov[2], and Dagmar Gerthsen[2] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Laboratorium für Elektronenmikroskopie, Karlsruher Institut für Technologie, 76128 Karlsruhe, Germany

ZnO is a wide gap semiconductor which attracted a renewed attention as a material for possible spintronic applications after Dietl *et al.* calculated Curie temperatures above room temperature for transition metal doped ZnO [1].

(Zn,Mn)O thin films were prepared by radio frequency magnetron sputtering on $Al_2O_3(0001)$ and $SiO_2/Si(100)$ substrates from a composite, partially oxidized ZnMn target. Sputtering was performed in Ar or N_2, since nitrogen is considered to enhance ferromagnetism in the (Zn,Mn)O system [2]. Structural properties were investigated by different techniques of transmission electron microscopy and X-ray diffraction. The formation of at least one secondary phase in samples with high Mn content could be observed, which had significant influence on the magnetic properties as shown by magnetization measurements. Ferromagnetism and exchange bias were observed in samples with high Mn concentration, suggesting the presence not only of a ferromagnetic, but also of an antiferromagnetic phase.

[1] T. Dietl *et al.*, Science **287**, 1019 (2000).
[2] K. R. Kittilstved *et al.*, Nat. Mater. **5**, 291 (2006).

MA 29.6 Thu 16:30 H22

Analysis of electric dipolar and quadrupolar transitions in X-ray absorption spectroscopy for Co doped ZnO — •Mehmet Kaya, Andreas Ney, Carolin Antoniak, and Heiko Wende — Fakultät für Physik and CeNIDE, Universität Duisburg-Essen, Duisburg, Germany

Co doped ZnO (Co:ZnO) is a promising candidate for dilute magnetic semiconductor devices. To realize a practical device, it is essential that a magnetic order is present above room temperature. Co:ZnO has been intensively investigated and there exist controversial results regarding its magnetic behavior. The authors in [1] report an absence of intrinsic ferromagnetic interactions of isolated and paired Co dopant atoms in Co:ZnO.

For optimum magnetic properties the analysis of the local structure is vital. The local structure can be studied by the linear dichroism in the X-ray absorption spectroscopy. We present an ab-initio study of XANES spectra of Co:ZnO using self-consistent potentials and full multiple scattering calculations. The calculations were made using the FEFF 8.4 code [2]. The results show a good agreement to experimental data. We present also an analysis of electric dipolar and quadrupolar transitions in the calculated spectra by comparison with the angular momentum resolved density of states. Furthermore our calculations will be compared to simulations obtained with the FDMNES code [3].

[1] Ney, A., et al. Phys. Rev. Lett. 100, 157201, (2008).
[2] Ankudinov, A. L., et al. Phys. Rev. B. 58, 7565, (1998).
[3] Joly, Y. Phys. Rev. B. 63, 125120, (2001).