#### **ABSTRACTS\***

#### (english language)

#### of Assoc. Prof. Iliana Apostolova

Presented for participation in a competition for occupying the academic position "professor"at the Department of Mathematics, physics and informatics, Field of higher education **4.** Natural sciences, mathematics and informatics, Professional field **4.1.** Physical sciences, Scientific specialty "Electrical, magnetic and optical properties of condensed matter (multiferroic properties of bulk samples and nanomaterials)", in the discipline "Physics with biophysics", published in the State newspaper, issue 102 /8.12.2023 and publication on the website of University of Forestry,

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\* The numbering of sections and publications is in accordance with Annex 2

B4. Habilitation thesis - scientific publications in editions that are referenced and indexed in worldwide databases of scientific information (Web of Science μ Scopus) (Magnetoelectric interactions in bulk samples and nanostructures - 11 publications).

B4.1. I. N. Apostolova, A. T. Apostolov, J. M. Wesselinowa, Theoretical study of the multiferroic properties of DyFeWO<sub>6</sub>, European Physical Journal B <u>95</u>, 133 (2022). ISSN (Print) 1434-6028, ISSN (Online) 1434-6036, Q<sub>3</sub>, SJR 0,4, IF 1,6 doi: 10.1140/epjb/s10051-022-00396-9

Abstract:

Magnetization M, specific heat Cp, polarization P and dielectric constant  $\epsilon$  of DyFeWO<sub>6</sub> are investigated for the first time using a microscopic model and the Green's function technique. The magnetic field dependence of M for temperatures below and above  $T_N$  is observed. Cp shows an anomaly at the Neel temperature  $T_N$  which disappears by applying an external magnetic field h. Pdecreases with increasing h. The antiferromagnetic transition in DyFeWO<sub>6</sub> is accompanied by a peak in  $\epsilon$ . With increasing magnetic field the peak decreases, shifts to smaller  $T_N$  values, and for strong magnetic fields vanishes. The magnetic field behaviour of P and  $\epsilon$  is an evidence for the multiferroicity of DyFeWO<sub>6</sub>. The observed results are in good qualitative agreement with the existing experimental data.

#### B4.2. A. T. Apostolov, I. N. Apostolova, J. M. Wesselinowa, Origin of multiferroism in Sm<sub>2</sub>BaCuO<sub>5</sub>, Solid State Communications <u>352</u>, 114808 (2022). ISSN 0038-1098, Q<sub>3</sub>, SJR 0,41, IF 2,1 doi: 10.1016/j.ssc.2022.114808

#### Abstract:

Proposing a microscopic model we have investigated the multiferroic properties of Sm<sub>2</sub>BaCuO<sub>5</sub>. The heat capacity shows two peaks at the antiferromagnetic transitions temperatures  $T_{NI} \sim 5$  K and  $T_{N2} \sim 23$  K. For the appearing of the extraordinary polarization  $\Delta P$  in Sm<sub>2</sub>BaCuO<sub>5</sub> we have considered the single-ion magnetostriction mechanism.  $\Delta P$  is zero without magnetic field. An external magnetic field h induces an electric polarization  $\Delta P$  below  $T_{N2}$  which varies linearly with h showing a linear magnetoelectric effect. Below  $T_{NI} \Delta P$  decreases due to ordering of the Sm-sublattice. There are some discrepancies in the experimental data for  $\Delta P(T, h)$  which we will try to clarify. In addition, the temperature and magnetic field dependence of the dielectric constant is discussed. The observed maximum value of the peak at  $T_{N2}$  shifts to smaller temperature values and increases with increasing external magnetic field.

### B4.3. I. N. Apostolova, A. T. Apostolov, J. M. Wesselinowa, Origin of multiferroism of $\beta$ -NaFeO<sub>2</sub>, Magnetochemistry <u>8</u>, 104 (2022). ISSN 2312-7481, Q<sub>2</sub>, SJR 0,43, IF 2,7 doi: 10.3390/magnetochemistry8090104

#### Abstract:

The multiferroic  $\beta$ -NaFeO<sub>2</sub> is theoretically investigated for the first time using a microscopic model and Green's function technique. A small room-temperature ferromagnetism is observed, which could be explained by canting of the antiferromagnetic sublattices. The ferromagnetic behaviour can be applied to applications in spintronic devices. We have investigated the temperature and magnetic field dependence of the spontaneous polarization  $P_S$ , as calculated from the transverse Ising model and the spin-assisted polarization  $\Delta P$  due to magnetostriction and antisymmetric Dzyaloshinsky–Moriya interactions. The influence of external magnetic fields along the y and z axis is discussed. This is indirect evidence for the multiferroic behaviour of NaFeO<sub>2</sub>. The temperature dependence of the relative dielectric permittivity is calculated.

#### B4.4. A. T. Apostolov, I. N. Apostolova, S. Trimper and J. M. Wesselinowa, Antiferroelectricity and weak ferromagnetism in rare earth doped multiferroic BiFeO<sub>3</sub>, Solid State Communications <u>300</u>, 113692 (2019).

#### ISSN 0038-1098, Q<sub>3</sub>, SJR 0,41, IF 1,521(2019) doi: 10.1016/j.ssc.2019.113692

#### Abstract:

The remanent polarization  $P_r$  and remanent magnetization  $M_r$  for different Sm-concentrations x in Smdoped BiFeO<sub>3</sub> is investigated using a microscopic model and the Green's function technique. For pure BiFeO<sub>3</sub> with a rhombohedral symmetry we obtain a hysteresis loop P(E) which is typical for a ferroelectric material. Further increase of x (x = 0.16) leads to a double hysteresis loop, which is typical for an antiferroelectric substance. Sm substitution induces a weak ferromagnetic moment at room-

temperature.  $P_r$  and  $M_r$  versus x show a maximum at x = 0.05. The ferroelectric phase transition temperature  $T_c$  decreases strongly whereas the magnetic phase transition temperature  $T_N$  increases slightly with increasing the Sm concentration x.

## B4.5. I. N. Apostolova, A. T. Apostolov and J. M. Wesselinowa, Room temperature ferromagnetism in multiferroic BaCoF<sub>4</sub> thin films due to surface, substrate and ion doping effects, Thin Solid Films <u>722</u>, 138567 (2021).

#### ISSN 0040-6090, Q<sub>2</sub>, SJR 0,47 IF 2,358(2021) doi: 10.1016/j.tsf.2021.138567

#### Abstract:

Using a microscopic model and the Green's function technique we have studied the influence of different surface, size and substrate effects on the magnetic properties of  $BaCoF_4$  thin films. The magnetization and the magnetic phase transition temperature increase for a compressible substrate  $Al_2O_3$ , whereas they decrease for a tensile substrate such as MgO. The film thickness influences also the magnetic properties. We have discussed a competition, a concurrence between the surface and substrate effects. Doping of bulk  $BaCoF_4$  with Al ions leads to weak room temperature ferromagnetism. Due to the magnetoelectric coupling is obtained that the polarization increases with increasing external magnetic field.

## B4.6. A. T. Apostolov, I. N. Apostolova, J. M. Wesselinowa, Substrate and doping effects on the multiferroic properties and the band gap of Bi<sub>2</sub>FeCrO<sub>6</sub> thin films, Thin Solid Films <u>739</u>, 138977 (2021). ISSN 0040-6090, Q2, SJR 0,47, IF 2,358 doi: 0.1016/j.tsf.2021.138977

#### Abstract:

The temperature, size and magnetic field dependence of the magnetization M, polarization P and band gap energy in double perovskite Bi<sub>2</sub>FeCrO<sub>6</sub> thin films are calculated on the basis of a microscopic model. The surface and substrate effects are discussed. P shows an anomaly at the Neel temperature  $T_N$ indicating a strong magnetoelectric coupling. There is a polarization anisotropy. An external magnetic field enhances the polarization and the kink at  $T_N$  disappears. M and P increase or decrease with decreasing film thickness by substrates which lead to compressive or tensile strains, respectively. Increase of M is also obtained by La ion doping of Bi<sub>2</sub>FeCrO<sub>6</sub> which leads to a compressive strain. We have calculated the band gap in dependence on substrate and doping effects.

#### B4.7. I. N. Apostolova, A. T. Apostolov and J. M. Wesselinowa, Electric, dielectric and magnetic properties of Ga, Er and Zn ion doped Fe<sub>2</sub>O<sub>3</sub> thin films, Physics Letters A <u>393</u>, 127167 (2021). ISSN 0375-9601, Q2, SJR 0,51, IF 2,707 doi:10.1016/j.physleta.2021.127167

#### Abstract:

Using a microscopic model we have investigated the electric, dielectric and magnetic properties of Ga, Er and Zn doped  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> thin films. The polarization P in Ga doped  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> decreases with increasing Ga content x, and increases with enhancing magnetic field h and decreasing film thickness N. In Ga doped hematite the dielectric constant  $\epsilon$  shows a peak at  $T_{C}$ .  $\epsilon$  decreases with increasing h, indicating a strong magneto-dielectric effect. The contributions of the spin-phonon and phonon-phonon interactions below and above  $T_c$  are considered. The dielectric constant in Ga, Er and Zn ion doped Fe<sub>2</sub>O<sub>3</sub> can increase or decrease for different ions and different ion doping concentration. The ion doping dependence of the magnetization is also calculated.

#### B4.8. I. N. Apostolova, A. T. Apostolov and J. M. Wesselinowa, Multiferroic properties of pure and ion doped BiCrO<sub>3</sub> - bulk and thin films, Physica Status Solidi B: Basic Solid State Physics 259(11), 2200171 (2022).

ISSN (Print) 0370-1972, ISSN (Online) 1521-3951, Q<sub>3</sub>, SJR 0,41, IF 1,6 doi: 10.1002/pssb.202200171

#### **Abstract:**

The multiferroic properties of  $BiCrO_3$  (BCO) bulk and thin films are investigated for the first time using a microscopic model. The influence of ion doping on the multiferroic properties of BCO is also studied because the doping process changes the physical properties and can be used for potential applications in magnetoelectronic devices. The magnetization M increases by Mn and decreases by Gaion doping whereas the Néel temperature  $T_N$  decreases in both cases. There are some discrepancies by polarization whether it is ferroelectric or antiferroelectric. It is shown that bulk pure BCO is antiferroelectric because the electric field dependence of polarization P shows a double hysteresis loop and the dielectric constant has no anomalies at  $T_N$ . In Ga-, Mn- or Ti-doped BCO a ferroelectric polarization appears. The specific heat shows a peak at  $T_N$  for BCO. By Ga doping, this peak vanishes with increasing x. The multiferroic behavior of BCO is demonstrated in the magnetic field dependence of the dielectric constant. In BCO thin films, ferroelectric and ferromagnetic behavior is observed.

#### B4.9. A. T. Apostolov, I. N. Apostolova, J. M. Wesselinowa, Size, external fields and ion doping effects on the multiferroic properties of hexagonal YMnO<sub>3</sub> nanoparticles, Materials Today Communications <u>30</u>, 103123 (2022).

ISSN 2352-4928, Q<sub>2</sub>, SJR 0,62, IF 3,8 doi: 10.1016/j.mtcomm.2022.103123

#### Abstract:

The size, external field and doping dependence of different properties of hexagonal YMnO<sub>3</sub> nanoparticles (NPs) is theoretically investigated. The spontaneous magnetization  $M_s$  increases with increasing electric field and decreasing NP size N. The polarization decreases with increasing magnetic field h. The band gap increases with decreasing N. The phonon mode  $\omega_0 = 167 \text{ cm}^{-1}$  shows a kink at  $T_N$ due to strong spin-phonon interaction. Applying h the kink disappears. By doping with different ions at

the Mn site, due to the observed different strains  $M_s$  can increase or decrease. By large Ti ion doping, above a critical x value, is taken into account that there appears a hexagonal-orthorhombic phase transition. The Gd and Sr substitution on the Y place in YMnO<sub>3</sub> NPs is also discussed. The dielectric function as a function of temperature, NP size and h is studied. The electron and phonon contributions to the specific heat Cp are shown.

B4.10. I. N. Apostolova, A. T. Apostolov, S. Trimper and J. M. Wesselinowa, Multiferroic Properties of Pure, Transition Metal, and Rare Earth–Doped BaFe<sub>12</sub>O<sub>19</sub> Nanoparticles,

#### Physica Status Solidi B: Basic Solid State Physics <u>258</u>(7), 2100069 (2021). ISSN (Print) 0370-1972, ISSN (Online) 1521-3951 Q<sub>3</sub>, SJR 0,41, IF 1,782 doi: 10.1002/pssb.202100069

#### Abstract:

Different properties of pure and Ni, Zr, and Sm-doped  $BaFe_{12}O_{19}$  bulk and nanoparticles are investigated using a microscopic model and the Green's function technique. The magnetization  $M_s$  increases whereas the coercive field  $H_c$  decreases with increasing particle size. The doping leads to a

decrease of  $M_s$  and the bandgap energy Eg with increasing Zr concentration x due to tensile strain and

to an increase of  $M_s$  and Eg after Ni doping due to compressive strain as well as due to size effects. The behavior of the spontaneous polarization  $P_s$  and the real part  $\epsilon'$  of the dielectric constant is opposite. The  $\epsilon'$  of a pure BaFe<sub>12</sub>O<sub>19</sub> nanoparticle decreases with increasing magnetic field *h*. The effects of Sm

substitution at Ba or Fe sites on  $\epsilon'$  and  $M_s$  are also studied.

### B4.11. A. T. Apostolov, I. N. Apostolova, S. Trimper and J. M. Wesselinowa, Physical Origin of Magnetoelectroporation, Physica Status Solidi B: Basic Solid State Physics <u>260</u>(3), 2200523 (2023).

ISSN (Print) 0370-1972, ISSN (Online) 1521-3951, Q<sub>3</sub>, SJR 0,41, IF 1,6(2022) doi: 10.1002/pssb.202200523

#### Abstract:

Magnetoelectroporation is an effective method of opening nanopores in cell membranes using magnetoelectric nanoparticles (MENPs) for the purpose of in vivo and in vitro delivery of drug substances to cancer cells. A microscopic approach is proposed as theoretical basis for that phenomenon. The underlying Hamiltonian includes the magnetic and ferroelectric subsystems characterized by two-order parameters. The related magnetoelectric coefficient  $\alpha_{\text{HE}}$  characterizes the relationship between the applied magnetic field and a generated local electric field. Whereas the spontaneous polarization  $P_S$  of the MENP is due to the arrangement of electric dipoles, there appears an additional spin-assisted polarization  $\Delta P$  owing to the magnetic phase transition. It is shown that the main contribution to the local field comes from  $P_S$ . Moreover, the local electric field depends on the orientation of the easy-axis magnetization of the MENPs with respect to applied external magnetic field. The magnetoelectric coefficient exhibits a nonlinear dependence on the external magnetic field. The results are based on an analytical Green's function method. The numerical calculations are performed for spherical, structurally heterogeneous nanoparticles composed on a core and a shell, where the noninteracting nanoparticles have the same diameter of 25 nm. The results are in qualitative agreement with experimental observations.

### G7. Scientific publications in editions that are referenced and indexed in worldwide databases with scientific information (Web of Science and SCOPUS), outside of the habilitation thesis (47 publications).

Γ7.1. A. T. Apostolov, I. N. Apostolova, S. G. Bahoosh, S. Trimper and J. M. Wesselinowa, Enhancement of the magnetoelectric effect in doped BaTiO<sub>3</sub> nanoparticles, Physica Status Solidi B: Basic Solid State Physics <u>252</u>(8), 1839 (2015).
ISSN (Print) 0370-1972, ISSN (Online) 1521-3951, Q<sub>2</sub>, SJR 0,665, IF 1,522 doi: 10.1002/pssb.201451752

#### Abstract:

Experimentally the polarization P and the magnetization M of BaTiO<sub>3</sub> (BTO) nanoparticles are altered under doping with transition metals as Fe-ions. Using a modified spin model for the magnetic and the ferroelectric part as well as the magnetoelectric coupling we have calculated the dependence of M and P on the Fe-doping content in BTO nanoparticles. The ferroelectric and ferromagnetic phase transition temperatures,  $T_{\rm C}^{\rm fe}$  and  $T_{\rm C}^{\rm fm}$  are likewise shifted due to doping. Owing to surface effects the influence of doping could be stronger compared to the bulk behavior. Whereas M and  $T_{\rm C}^{\rm fm}$  increase with increasing Fe-ion concentration, P and  $T_{\rm C}^{\rm fe}$  decrease if the dopant concentration is enhanced.

### **Γ7.2. I. N. Apostolova, A. T. Apostolov, S. G. Bahoosh, S. Trimper and J. M. Wesselinowa,** Origin of multiferroism in the charge frustrated LuFe<sub>2</sub>O<sub>4</sub> compound, Physics Letters A <u>379</u>(7), 743-746 (2015).

ISSN (Print) 0375-9601, ISSN (Online) 1873-2429, Q<sub>2</sub>, SJR 0,663, IF 1,677 doi: 10.1016/j.physleta.2014.12.043

#### Abstract:

We propose a microscopic model in order to study the multiferroic properties of LuFe<sub>2</sub>O<sub>4</sub>. It is shown that the real part of the dielectric constant  $\epsilon'$  has a plateau near the magnetic phase transition  $T_N = 240$  K. At room temperature  $\epsilon'$  decreases strongly by applying an external magnetic field *H*. This behavior is an evidence for a strong coupling of spins and electric dipoles in agreement with the experimental data. The observed kinks in the temperature dependence of the phonon energy and damping for the  $E_g^3$  mode around the ferroelectric and ferrimagnetic transition temperatures show that this phonon mode is closely related to the structural, magnetic and ferroelectric properties of LuFe<sub>2</sub>O<sub>4</sub>.

Γ7.3. A. T. Apostolov, I. N. Apostolova, S. G. Bahoosh, S. Trimper, M. T. Georgieva and J. M. Wesselinowa, Multiferroic properties of S = 1/2 chain cuprates LiCuVO<sub>4</sub>. Comparison with LiCu<sub>2</sub>O<sub>2</sub>, Modern Physics Letters B <u>29</u>(17), 1550086 (2015). ISSN (print) 0217-9849, ISSN (online) 1793-6640, Q<sub>3</sub>, SJR 0,248, IF 0,547 doi: 10.1142/S0217984915500864

#### Abstract:

We propose a microscopic model in order to study the multiferroic (MF) properties of LiCuVO<sub>4</sub> (LCVO) taking into account the competing nearest and next-nearest magnetic interactions, frustration and a linear magnetoelectric (ME) coupling. We obtain for  $\alpha = |J_2/J_1| = 0.76$ . The temperature and magnetic field dependence of the polarization  $P_a$  and  $P_c$  is observed. It is shown that the dielectric constant  $\epsilon_a$  has a kink near the magnetic phase transition  $T_N = 2.4$  K which disappears with increasing of the external magnetic field. Some differences in the MF behavior between LiCu<sub>2</sub>O<sub>2</sub> (LCO) and LCVO are discussed.

Γ7.4. I. N. Apostolova, A. T. Apostolov, J. M. Wesselinowa and S. Trimper, Magnetic and dielectric properties of S = 1/2 chain cuprate Li<sub>2</sub>ZrCuO<sub>4</sub>, Physica Status Solidi B: Basic Solid State Physics <u>252</u>(12), 2667 (2015).

ISSN (Print) 0370-1972, ISSN (Online) 1521-3951, Q<sub>2</sub>, SJR 0,665, IF 1,522 doi: 10.1002/pssb.201552311

#### Abstract:

We propose a microscopic model in order to study the multiferroic properties of Li<sub>2</sub>ZrCuO<sub>4</sub> at low temperatures taking into account the competing nearest and next-nearest magnetic interactions, frustration, and a linear magnetoelectric coupling. To understand the experimental observation an antiferroelectric interaction between the CuO<sub>2</sub> chains is included. The magnetization M(T) exhibits a peak at the antiferromagnetic transition temperature  $T_N$ , whereas the dielectric function  $\epsilon_a(T, H_a)$  offers no anomaly at that temperature, however  $\epsilon$  can be governed by an external magnetic field  $H_a$ . It decreases with increasing magnetic field  $H_a$ . Our analysis provides no indication about a glass-like order of Li discussed controversially.

# Γ7.5. A. T. Apostolov, I. N. Apostolova and J. M. Wesselinowa, Microscopic approach to the magnetoelectric coupling in *R*CrO<sub>3</sub>, Modern Physics Letters B <u>29</u>(1), 1550251 (2015). ISSN (print) 0217-9849, ISSN (online) 1793-6640, Q<sub>3</sub>, SJR 0,248, IF 0,547 doi: 10.1142/S0217984915502516

Abstract:

A microscopic model is proposed to describing the multiferroic properties in  $RCrO_3$ , where R is the

magnetic rare earth ion. Using the Green's function theory, the weak ferromagnetism and the coercive field are calculated by a balance between the Dzyaloshinskii–Moriya interaction (DMI), the single-ion anisotropy and the exchange interaction. We have discussed the magnetic rotational spin-reorientation (SR) transition between  $\Gamma_4$  and  $\Gamma_2$  phases in SmCrO<sub>3</sub> and the abrupt one between  $\Gamma_4$  and  $\Gamma_1$  in ErCrO<sub>3</sub> calculating the energies in the corresponding phases. The type of the phase transition in *R*CrO<sub>3</sub> is determined by the sign of the second magnetic anisotropy constant. In order to investigate the origin of the extraordinary ferroelectricity in *R*CrO<sub>3</sub>, we have studied the different contributions in the polarization due to the antisymmetric exchange DMI and the magnetostriction arising from the Crordering. It is shown that the polarization is due to the interaction between the magnetic *R*- and Cr-ions. The influence of a magnetic field on the polarization and of an electric field on the magnetization are also calculated as an evidence for a strong magnetoelectric coupling in *R*CrO<sub>3</sub>.

# Γ7.6. A. T. Apostolov, I. N. Apostolova and J. M. Wesselinowa, Theory of magnetic field control on polarization in multiferroic *R*CrO<sub>3</sub> compounds, European Physical Journal B <u>88</u>, 328 (2015). ISSN (Print) 1434-6028, ISSN (Online) 1434-6036, Q<sub>2</sub>, SJR 0,514, IF 1,223 doi: 10.1140/epjb/e2015-60649-4

#### Abstract:

A microscopic mechanism to describe the magnetic field H dependence of the polarization P is proposed on the basis of a microscopic model for  $RCrO_3$  including the spin-phonon interaction. Using the Green's function theory in Peierls systems we have studied the two contributions to P due to the antisymmetric exchange Dzyaloshinskii-Moriya interaction  $P_{AS}$  and the magnetostriction  $P_{MS}$ . The behaviour of P(H) – increase or decrease – in different multiferroics can be explained in our model taking into account the second order spin-phonon interaction constants. When a magnetic field is applied to a magnetoelectric material, the material is strained. H changes the average of the spin operator products and so P. Moreover, H renormalizes the elastic constant which explains the strain effect. From here we have found a qualitative relationship between pressure and magnetic field effects on P. The observed results are in good qualitatively agreement with the experimental data.

## **Γ7.7. A. T. Apostolov, I. N. Apostolova, S. Trimper and J. M. Wesselinowa, Magnetoelectric coupling and spin reorientation in BiFeO<sub>3</sub>, Physical Status Solidi B: Basic Solid State Physics <u>254</u>(4), 1600433 (2016).**

ISSN (Print) 0370-1972, ISSN (Online) 1521-3951, Q<sub>1</sub>, SJR 0,96, IF 1,674 doi: 10.1002/pssb.201600433

#### Abstract:

We have studied the electric properties of multiferroic BiFeO<sub>3</sub> (BFO) using the transverse Ising model in terms of pseudo-spin variables *S* with S = 7/2 and the Green's function method. Mechanisms of magnetoelectric (ME) couplings and electric field-induced spin-reorientation (SR) transition in BFO (71° in-plane and 109° out-of-plane switching) are examined. It is established that the spontaneous polarization  $P_S$  is responsible for the origin of an incommensurate non-collinear magnetic phase below  $T_N$ . The relevance of two types of ME mechanisms is shown: the first one is quadratic with respect to the magnetic spins and the ferroelectric variables, whereas a second one defines a ME interaction which is induced from the appearance of a spontaneous polarization in BFO, called antisymmetric ME interaction. When an external magnetic field is applied they compete against each other and as a result the spontaneous polarization  $P_S$  is renormalized. The extraordinary polarization below  $T_N$  is numerically calculated and its dependency on the easy-axis anisotropy *K* and the external magnetic field is examined. The type of magnetic SR transition under the influence of the electric field is determined. The critical values of *E* for different switching processes are numerically calculated.

## **F7.8.** A. T. Apostolov, I. N. Apostolova and J. M. Wesselinowa, Influence of spin-phonon interactions and spin-reorientation transitions on the phonon properties of $RCrO_3$ , Modern Physics Letters B <u>31</u>(03), 1750009 (2017).

ISSN (print) 0217-9849, ISSN (online) 1793-6640, Q<sub>4</sub>, SJR 0,226, IF 0,731 doi: 10.1142/S0217984917500099

#### Abstract:

Using a microscopic model and a Green's function technique we calculate the renormalized phonon energy in multiferroic  $RCrO_3$  (R = Sm, Dy, Er, Pr, Gd and Y) compounds as a function of temperature, magnetic field and R-ionic radius. We explain the observed anomalies in the temperature dependence of the phonon spectra based on a detailed analysis of the influence of the magnetic sublattices, the interaction between them and the spin-reorientation (SR) transition on lattice vibrations via spinphonon interactions. When the rare earth ions are magnetic we investigate their essential role for the anomalies around the SR temperature. For the case when R is nonmagnetic, for example YCrO<sub>3</sub>, we propose a new microscopic model. We define an induced Dzyaloshinskii–Moriya (IDM) vector as a consequence from the spontaneous polarization. This IDM interaction is responsible for the appearance of a temperature-driven SR transition, which itself is responsible for the phonon anomalies at low temperatures. The numerical calculations are in good qualitative agreement with the experimental data.

## **F7.9.** A. T. Apostolov, I. N. Apostolova, S. Trimper and J. M. Wesselinowa, Room temperature ferromagnetism in pure and ion doped $SnO_2$ nanoparticles, Modern Physics Letters B, <u>31</u>(36) 1750351 (2017).

ISSN (print) 0217-9849, ISSN (online) 1793-6640, Q<sub>4</sub>, SJR 0,226, IF 0,731 doi: 10.1142/S0217984917503511

#### Abstract:

Using a microscopic model taking into account the spin-phonon interactions we have studied the magnetic properties of pure and ion-doped  $\text{SnO}_2$  nanoparticles (NPs). The magnetization M in pure  $\text{SnO}_2$  NPs is due to surface oxygen vacancies. By doping with magnetic Co ion we observe a maximum in M for small Co-concentration, x = 1%, whereas for nonmagnetic Cu ion M increases with x. By Co-doping there is a local distribution for small Co-concentration, whereas by Cu this is not the case. It is shown that there is a strong connection between the lattice and M. The results are in good agreement with the experimental data.

## Γ7.10. A. T. Apostolov, I. N. Apostolova, S. Trimper and J. M. Wesselinowa, Dielectric properties of multiferroic CuCrO<sub>2</sub>, European Physical Journal B <u>90</u>, 236 (2017). ISSN (Print) 1434-6028, ISSN (Online) 1434-6036, Q<sub>2</sub>, SJR 0,43, IF 1,536 doi: 10.1140/epjb/e2017-80461-4

#### Abstract:

We propose a microscopic model in order to study the multiferroic properties of the triangular compound CuCrO<sub>2</sub> taking into account antiferromagnetic interactions in the *ab* plane, spin-phonon interactions and quadratic magnetoelectric (ME) coupling. The temperature and magnetic field dependence of the polarization  $P_{ab}$  and dielectric constant  $\epsilon_{ab}$  is calculated.  $P_{ab}$  increases when *h* is parallel to its direction and decreases when *h* is perpendicular to it. We show that  $\epsilon_{ab}$  has a kink near the magnetic phase transition  $T_N = 24$  K which disappears with increasing of an external magnetic field *h<sub>ab</sub>*. This behavior is an evidence for a strong ME coupling and in qualitative agreement with the experimental data.

## Γ7.11. A. T. Apostolov, I. N. Apostolova and J. M. Wesselinowa, $La_{1-x}Sr_xMnO_3$ nanoparticles for magnetic hyperthermia, Physica Status Solidi B: Basic Solid State Physics 255(6), 1700587 (2018).

### ISSN (Print) 0370-1972, ISSN (Online) 1521-3951, Q<sub>2</sub>, SJR 0,519, IF 1,454 doi: 10.1002/pssb.201700587

#### Abstract:

Using a modified Heisenberg model and a Green's function technique we have studied the influence of size d and concentration x of Sr dopants on the Curie temperature  $T_C$ , saturation magnetization  $M_S$ , coercivity  $H_C$  and specific absorption rate (SAR) of single-domain La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3</sub> nanoparticles. Their magnetic properties are explained based on the "magnetically death" surface layer and the competition between the ferromagnetic double-exchange and antiferromagnetic super-exchange interaction. We

calculated the specific absorption rate which characterizes the efficiency of the absorption energy when the magnetic hyperthermia is applied as a therapeutic method for the treatment of tumors. A set of nanoparticles appropriate for in vivo and in vitro medical applications, such as magnetic hyperthermia and drug delivery to cancer cells, is determined. The established methodology and microscopic model are suitable to study the magnetic properties of low-dimensional systems (thin films and nanoparticles) such as La<sub>1x</sub>A<sub>x</sub>MnO<sub>3</sub> with A = Ca, Ag, Ba, Na for medical applications.

## **Γ7.12.** A. T. Apostolov, I. N. Apostolova and J. M. Wesselinowa, A comparative study of the magnetization in transition metal ion doped CeO<sub>2</sub>, TiO<sub>2</sub> and SnO<sub>2</sub> nanoparticles, Physica E: Low-dimensional Systems and Nanostructures <u>99</u>, 202 (2018).

#### ISSN 1386-9477, Q<sub>2</sub>, SJR 0,538, IF 3,176 doi: 10.1016/j.physe.2018.02.007

#### Abstract:

Using the microscopic s–d model taking into account anharmonic spin-phonon interactions we have studied the magnetic properties of Co and Cu ion doped CeO<sub>2</sub> and TiO<sub>2</sub> nanoparticles and compared them with those of SnO<sub>2</sub>. By Co-doping there is a maximum in the magnetization M(x) curve for all nanoparticles observed in the most transition metal doped ones. The s–d interaction plays an important role by the decrease of M at higher dopant concentration. We have discussed the magnetization in dependence of different model parameters. By small Cu-ion doping there are some differences. In CeO<sub>2</sub> M decreases with the Cu-concentration, whereas in TiO<sub>2</sub> and SnO<sub>2</sub> M increases. For higher Cu dopant concentrations M(x) decreases in TiO<sub>2</sub> nanoparticles. We obtain room temperature ferromagnetism also in Zn doped CeO<sub>2</sub>, TiO<sub>2</sub> and SnO<sub>2</sub> nanoparticles is due to a combination effect of multivalent metal ions, oxygen vacancies, different radius of cation dopants, connection between lattice and magnetism, as well as competition between the s–d and d–d ferromagnetic or antiferromagnetic interactions.

# **Γ7.13.** A. T. Apostolov, I. N. Apostolova and J. M. Wesselinowa, Theoretical study of room temperature ferromagnetism and band gap energy of pure and ion doped In<sub>2</sub>O<sub>3</sub> nanoparticles, Journal of Magnetism and Magnetic Materials <u>456</u>, 263 (2018). ISSN 0304-8853, Q<sub>2</sub>, SJR 0,68, IF 2,683 doi: 10.1016/j.jmmm.2018.02.045

#### Abstract:

Using the s-d microscopic model including the electron-phonon interaction and the Green's function theory we have considered the origin of room temperature ferromagnetism (RTFM) in pure and ion doped  $In_2O_3$  nanoparticles (NPs). The magnetization *M* increases with decreasing particle size. *M* of Fe, Tb and Mn doped  $In_2O_3$  NPs is investigated, which increases, decreases and has a maximum, respectively, with increasing doping concentration. The RTFM is due to surface oxygen vacancies and different ionic radius of the dopants compared to that of the host ions. This differences lead to different strains which changes the exchange interaction constants. We have calculated the dependence of the band gap energyon the particle size in  $In_2O_3$  NPs and the Fe concentration of Fe doped  $In_2O_3$  NPs. The results are in good qualitative agreement with the experimental data.

## **Γ7.14.** A. T. Apostolov, I. N. Apostolova and J. M. Wesselinowa, Theoretical study of the phonon properties of pure and ion doped CeO<sub>2</sub> nanoparticles, Solid State Communications <u>279</u>, 17 (2018). ISSN 0038-1098, Q<sub>2</sub>, SJR 0,45, IF 1,433 doi: 10.1016/j.ssc.2018.05.007

#### Abstract:

Using a microscopic model taking into account the spin-phonon interactions we have studied the phonon properties of pure and ion doped CeO<sub>2</sub> nanoparticles (NPs). The phonon energy  $\omega$  decreases whereas the damping  $\gamma$  increases with increasing temperature and decreasing particle size. Near the Curie temperature in the NPs there appears a kink in  $\omega(T)$  and  $\gamma(T)$ . The phonon properties are very sensitive especially to the anharmonic spin-phonon interaction. In dependence of the radius of the doping ions compared to the host ones  $\omega$  could be reduced (Pr, Sm, Nd, La) or enhanced (Co, Y, Cu). The changes of the lattice parameters lead to changes of the exchange interaction and anharmonic spin-

phonon interaction constants. The phonon damping is always enhanced by the doped NPs. It is shown that the changes in the phonon energy and damping of ion doped  $CeO_2$  NPs are due to combined effects of size, strain or defect effects.

## **F7.15.** A. T. Apostolov, I. N. Apostolova and J. M. Wesselinowa, Size and doping dependence of the phonon properties of $SnO_2$ nanopartocles, Modern Physics Letter B <u>32</u>(21), 1850250 (2018).

ISSN (print) 0217-9849, ISSN (online) 1793-6640, Q<sub>4</sub>, SJR 0,229, IF 0,929 doi: 10.1142/S0217984918502500

#### Abstract:

Using a microscopic model, taking into account the spin-phonon interactions and the Green's function technique, we have studied the phonon properties of pure and ion-doped SnO<sub>2</sub> nanoparticles (NPs). The phonon energy of SnO<sub>2</sub> NPs decreases whereas the damping increases with decreasing particle size. Near the Curie temperature in theNPs, there appears an anomaly in the phonon energy  $\omega(T)$  and damping  $\gamma(T)$ . The phonon properties are very sensitive to the anharmonic spin-phonon interaction *R*. They can increase or decrease for R > 0 or R < 0 with increasing of temperature, respectively. In dependence of the radius of the doping ions, the phonon energies  $\omega$  could be reduced (Co, Fe, Sm, Nd) or enhanced (Cu). The phonon damping is always enhanced in the doped NPs. In summary, due to the size and temperature effects, we obtain changes in the phonon energy and damping in pure SnO<sub>2</sub> NPs, whereas in ion-doped ones, the doping effects strengthen these properties.

## **F7.16.** A. T. Apostolov, I. N. Apostolova and J. M. Wesselinowa, Magnetic properties of rare earth-doped $\text{SnO}_2$ , TiO<sub>2</sub> and CeO<sub>2</sub> nanoparticles, Physica Status Solidi B: Basic Solid State Physics <u>255(8)</u>, 1800179 (2018).

ISSN (Print) 0370-1972, ISSN (Online) 1521-3951, Q<sub>2</sub>, SJR 0,519, IF 1,454 doi: 10.1002/pssb.201800179

#### Abstract:

The magnetic properties of rare earth doped  $SnO_2$ ,  $TiO_2$ , and  $CeO_2$  nanoparticles are studied theoretically. The discrepancies in the literature for some doping cases are explained, for example, the lattice parameters and the magnetization in Pr and Sm doped  $CeO_2$  nanoparticles. There is a strong connection between the lattice deformations and the magnetization M. M decreases (except for Y doped  $CeO_2$ ) due to the larger radius of the rare earth ions compared to that of the host ions which leads to increase of the lattice parameters and decrease of the exchange interactions. The decrease of M is due also to the enhanced number of oxygen vacancies with increasing dopant concentration. For Y doping the lattice parameters decrease and M increases with increasing Y concentration. We have discussed the origin of the different behavior of M in rare earth doped nanoparticles.

## Γ7.17. A. T. Apostolov, I. N. Apostolova and J. M. Wesselinowa, Ferroelectricity in the multiferroic delafossite CuFeO<sub>2</sub> induced by ion doping or magnetic field, Solid State Communications <u>292</u>, 11 (2019). ISSN 0038-1098, Q<sub>3</sub>, SJR 0,419, IF 1,521 doi: 10.1016/j.ssc.2019.01.014

Abstract:

On the basis of a microscopic model and using the Green's function technique we have studied the induced ferroelectric polarization  $P_{[110]}$  along the [110] direction in the triangular CuFeO<sub>2</sub>. It is shown that  $P_{[110]}$  is induced by an external magnetic field parallel to the *c* axis  $h_c$  or a nonmagnetic ion substitution which both can break the inversion symmetry of the system. Our Hamiltonian consists of Heisenberg antiferromagnetic interactions in and out of the *ab* plane and anharmonic spin-phonon interactions.  $P_{[110]}$  decreases with increasing the temperature *T*. It appears at  $T \sim 9$  K and begins to increase below  $T \sim 9$  K, which is the transition temperature to a noncollinear phase. This behavior is an evidence for the multiferroic character of CuFeO<sub>2</sub>. By doping with Rh ions the polarization has a maximum in the curve  $P_{[110]}(x)$  with increasing Rh concentration *x* whereas by Sc doping it decreases. The observed results are in qualitative agreement with the experimental data.

# Γ7.18. A. T. Apostolov, I. N. Apostolova and J. M. Wesselinowa, Specific absorption rate in Zn-doted ferrites for self-controlled magnetic hyperthermia, European Physical Journal B <u>92</u>, 58 (2019). ISSN (Print) 1434-6028, ISSN (Online) 1434-6036, Q<sub>2</sub>, SJR 0,459 IF 1,347 doi: 10.1140/epjb/e2019-90567-2

#### Abstract:

In this paper, we study mixed ferrites nanoparticles with structure formula  $Me_{1-x}Zn_xFe_2O_4$  (Me = Co, Ni, Cu, Mn) appropriated for self-controlled magnetic hyperthermia (SMHT) for in vivo and in vitro applications. We discuss in details the influence of the size *d*, the Zn-ion concentration *x* on the magnetic characteristics: saturation magnetization  $M_s$ , coercivity  $H_c$ , effective anisotropy  $K_{eff}$  and specific absorption rate (*SAR*). From a theoretical point of view we investigate monodispersed, non-interactive, single-domain spherical magnetic nanoparticles (MNPs). We propose a simple core–shell model with a constant thickness of the surface layer. We explain the behaviour of *SAR* as a function of size and dopping based on two thermal heating mechanisms: the mechanism leading to dynamic hysteresis loops of superparamagnetic origin and the heating mechanism via conventional metastable hysteresis. We investigate also a thermal heating efficiency based on the Zn-ion concentration. We show that whether *SAR* decreases (increases) when doping increases depends on whether the nanoparticle diameter *d* is smaller (larger) than the particle size  $d_{max}$  for which *SAR* has a maximum value. The numerical results are in qualitative agreement with many experimental data.

**Γ7.19.** A. T. Apostolov, I. N. Apostolova and J. M. Wesselinowa, Phonon properties of delafossite multiferroic compound CuFeO<sub>2</sub>. Comparison with CuCrO<sub>2</sub>, Modern Physics Letters B <u>33</u>(12), 1950141 (2019).

### ISSN (print) 0217-9849, ISSN (online) 1793-6640, Q<sub>3</sub>, SJR 0,258, IF 1,224 doi: 10.1142/S0217984919501410

#### Abstract:

The temperature, magnetic field and ion doping dependence of the phonon properties of CuFeO<sub>2</sub> are studied on the basis of a microscopic model and using Green's function technique. The phonon energy decreases with increasing temperature, whereas the phonon damping increases. There is a kink at the phase transition temperature  $T_{N1}$  which shows the influence of the magnetic field on the phonon properties. The kinks vanish by applying an external magnetic field. By doping of ions with different radius compared to the Fe ion, the phonon energy in CuFeO<sub>2</sub> can increase (Ga) or decrease (Sc) with increasing dopant concentration, whereas the damping is always enhanced. The results are compared with those of CuCrO<sub>2</sub>. Some discrepancies in the literature are discussed. The observed results are in qualitative agreement with the experimental data.

# **Γ7.20.** A. T. Apostolov, I. N. Apostolova and J. M. Wesselinowa, Magnetic and dielectric properties of pure and ion doped RCrO<sub>3</sub> nanoparticles, European Physical Journal B <u>92</u>, 105 (2019). ISSN (Print) 1434-6028, ISSN (Online) 1434-6036, Q<sub>2</sub>, SJR 0,459, IF 1,347 doi: 10.1140/epjb/e2019-100112-x

#### Abstract:

Using a microscopic model and the Green's function technique the magnetic and dielectric properties of YCrO<sub>3</sub> and GdCrO<sub>3</sub> nanoparticles (NPs) are studied and compared with the bulk properties. Due to different surface exchange interaction constants the magnetization in YCrO<sub>3</sub> increases whereas in GdCrO<sub>3</sub> decreases with decreasing particle size. The size dependence of the coercive field in GdCrO<sub>3</sub> NPs is also discussed. The bulk dielectric constant  $\epsilon'$  in YCrO<sub>3</sub> is smaller than that in NPs, whereas in GdCrO<sub>3</sub> is observed the opposite behavior. The magnetic field influences  $\epsilon'$  in YCrO<sub>3</sub> NPs which is an indirect evidence for a strong magnetoelectric coupling. The effects of ion doping on  $\epsilon'$  are also studied.

**Γ7.21.** A. T. Apostolov, I. N. Apostolova, S. Trimper and J. M. Wesselinowa, Origin of ferromagnetism in pure and ion doped pyrite FeS<sub>2</sub> nanoparticles, Physica Status Solidi B: Basic Solid State Physics <u>256(10)</u>, 1900201 (2019). ISSN (Print) 0370-1972, ISSN (Online) 1521-3951, Q<sub>2</sub>, SJR 0,504, IF 1,481

#### doi: 10.1002/pssb.201900201

#### Abstract:

It is demonstrated theoretically that the magnetization of  $FeS_2$  nanoparticles is originated by the appearance of sulfur vacancies at the surface, where  $FeS_2$  undergoes a reduction to FeS. This change is accompanied by a transition from the zero spin configuration of  $Fe^{2+}$  ions to a spin S = 2 state. Additionally there are uncompensated Fe spins on the surface. As result one observes ferromagnetism which is described using the Heisenberg model. The applied Green's function method allows calculating the magnetization of  $FeS_2$  nanoparticles versus the FeS concentration on the surface at finite temperature and for different particles sizes as well as the increase of the magnetization of  $FeS_2$  nanoparticles size. It is shown that Co ion doping can induce ferromagnetism in bulk  $FeS_2$  and enhance it in FeS\_2 nanoparticles.

Γ7.22. A. T. Apostolov, I. N. Apostolova and J. M. Wesselinowa, Dielectric Properties in Transition Metal and Rare-Earth-Doped Multiferroic BaTiO<sub>3</sub> Nanoparticles, Physica Status Solidi B: Basic Solid State Physics <u>257</u>(9), 2000046 (2020).
ISSN (Print) 0370-1972, ISSN (Online) 1521-3951, Q<sub>2</sub>, SJR 0,51, IF 1,710 doi: 10.1002/pssb.202000046

#### Abstract:

The temperature, doping concentration, size, and magnetic field dependences of the real part of the dielectric function  $\epsilon'$  for Fe and Er ion-doped BaTiO<sub>3</sub> — bulk and nanoparticles — are calculated using microscopic models and the Green's function technique. The Fe ions substitute the Ti ions and cause a tensile strain. The maximum value of  $\epsilon'$  and the ferroelectric phase transition temperature  $T_C$  decrease with increasing the Fe doping concentration. Moreover,  $\epsilon'$  decreases with decreasing particle size and increases with increasing an external magnetic field. The latter is an evidence for a strong magnetodielectric effect. By substituting the Ba with Er ions, there appears a strong compressive strain. It causes an increase in the maximum of  $\epsilon'$  and  $T_C$  with increasing the Er ion concentration.

# **Γ7.23.** A. T. Apostolov, I. N. Apostolova and J. M. Wesselinowa, Magnetic field effect on the dielectric properties of rare earth doped multiferroic BiFeO<sub>3</sub>, Journal of Magnetism and Magnetic Materials <u>513</u>, 167101 (2020). ISSN 0304-8853, Q<sub>2</sub>, SJR 0,665, IF 2,993 doi: 10.1016/j.jmmm.2020.167101

#### Abstract:

The temperature, doping concentration and magnetic field dependence of the dielectric constant in lanthanum doped barium titanate are studied using a microscopic model and the Green's function technique. A kink in the temperature dependence of the dielectric constant is observed near the Neel temperature. The Neel temperature and the ferroelectric transition temperature decrease with increasing doping concentration. The doping dependence of the dielectric constant shows a maximum value at 0.15. For small magnetic fields the dielectric constant increases strongly, whereas for stronger ones it begins to decrease slightly, i.e. there is a critical field for the transition from spiral cycloidal to antiferromagnetic spin arrangement.

#### **Γ7.24.** A. T. Apostolov, I. N. Apostolova and J. M. Wesselinowa, Co, Fe and Ni ion doped CeO<sub>2</sub> nanoparticles for application in magnetic hyperthermia, Journal: Physica E: Lowdimensional Systems and Nanostructures <u>124</u>, 114364 (2020). ISSN 1386-9477, Q<sub>2</sub>, SJR 0,581, IF 3,382 doi: 10.1016/j.physe.2020.114364

#### Abstract:

For magnetic hyperthermia (MHT) applications the magnetic nanoparticles (NPs) should have high saturation magnetization M, low coercive field  $H_C$ , Curie temperature  $T_C \approx 315$  K, size d < 20 nm and biocompatibility. M is very small in undoped CeO<sub>2</sub> NPs but doping with transition metal ions could enhance M. To observe an increase of M and a decrease of  $H_C$  the enhanced oxygen vacancies, the interaction between the Ce<sup>3+</sup> ions composed on the surface, and the exchange interactions between the Ce ions and the Co, Fe, Ni ions are considered. We have calculated selfconsistently the temperature, size, shape and doping ion concentration dependence of M,  $H_C$  and  $T_C$  in undoped and Co, Fe and Ni doped CeO<sub>2</sub> NPs using a microscopic model and the Green's function technique. In conclusion, appropriate for application in MHT could be Co, Fe and Ni doped spherical CeO<sub>2</sub> NPs with size of d =10 nm and doping concentration x = 0.07, 0.05 and 0.06, respectively. For these values the Curie temperature is observed as  $T_C = 315$  K.

#### Γ7.25. I. N. Apostolova, A. T. Apostolov and J. M. Wesselinowa, Multiferroic properties of pure and transition metal doped LaFeO<sub>3</sub> nanoparticles, Physica Status Solidi B: Basic Solid State Physics 258(2), 2000482 (2020).

ISSN (Print) 0370-1972, ISSN (Online) 1521-3951, Q<sub>2</sub>, SJR 0,51, IF 1,710 doi: 10.1002/pssb.202000482

#### Abstract:

The size, doping concentration, and magnetic field dependences of the magnetization M and the real part of the dielectric function ɛ' in doped LaFe<sub>1-x</sub>M<sub>x</sub>O<sub>3</sub> nanoparticles (NPs) are studied using a microscopic model. Although M increases,  $\varepsilon'$  decreases with decreasing NPs size in pure LaFeO<sub>3</sub>. Doping with different ions causes different strain which modifies the exchange interaction. As a consequence, M and  $\varepsilon'$  grow with increasing Mn or Zn ion doping, whereas both quantities decrease by doping with Ti or Al ions. The magneto-dielectric coefficient increases with an applied external magnetic field and Mn doping concentration in pure and Mn-doped LaFeO<sub>3</sub> indicating that pure and doped LaFeO<sub>3</sub> NPs exhibit a multiferroic behavior. A microscopic model is proposed to study multiferroic Bi<sub>2</sub>NiMnO<sub>6</sub> thin films.

#### Γ7.26. I. N. Apostolova, A. T. Apostolov and J. M. Wesselinowa, Multiferroic and phonon properties of pure and ion doped CoCr<sub>2</sub>O<sub>4</sub> - bulk and nanoparticles, Journal of Alloys and Compounds 852, 156885 (2021). ISSN 0925-8388, Q<sub>1</sub>, SJR 1,027, IF 6,371 doi:10.1016/j.jallcom.2020.156885

#### **Abstract:**

Using a microscopic model we have studied different properties of pure and ion doped  $CoCr_2O_4$  - bulk and nanoparticles (NPs). The magnetization  $M_s$  and the Curie temperature  $T_c$  decrease with decreasing particle size. By Fe doping  $M_S$  and  $T_C$  increase with enhancing Fe concentration x whereas by Mg doping we obtain the opposite effect. In the first case there is a compressive strain, in the second one - a tensile strain due to the different radii of the doping ions compared to the host ones. This leads to different exchange interaction constants in the doped states. The polarization  $P_S$  increases with increasing Fe doping concentration x. Two anomalies are observed in the specific heat  $C_P$ , at  $T_C = 98$  K, and  $T_s = 25$  K, which are not so sharp applying h. The temperature, magnetic field, size and doping dependence of the phonon energy  $\omega_0 = 685 \text{ cm}^{-1}$  and damping are also investigated.

#### Γ7.27. I. N. Apostolova, A. T. Apostolov and J. M. Wesselinowa, Differences in the multiferroic properties of AgCrS<sub>2</sub> and AgCrO<sub>2</sub>, Solid State Communications <u>323</u>, 114119 (2021). ISSN 0038-1098, Q<sub>3</sub>, SJR 0,413, IF 1,934 doi: 10.1016/j.ssc.2020.114119

### **Abstract:**

Using a microscopic model we have investigated the multiferroic properties of the triangular compound AgCrS<sub>2</sub> taking into account different exchange interactions in the CrS<sub>2</sub> layers and between them, spinphonon interactions and quadratic magnetoelectric coupling. By AgCrO<sub>2</sub> is taken into account also the single ion anisotropy. The ferroelectricity in AgCrS<sub>2</sub> can be explained by atomic displacements. It is a geometric ferroelectricity and can be described by the transverse Ising model. The polarization P shows a kink at  $T_N$  which disappears applying a magnetic field h. P in AgCrO<sub>2</sub> is a spin-driven one, the noncollinear spiral spin structure is responsible for the inversion symmetry breaking similar to that for CuCrO<sub>2</sub>. Both polarizations are described within different models. P in AgCrO<sub>2</sub> exists only below  $T_N$ and decreases with h. The temperature and magnetic field dependence of the dielectric constant are similar in both compound. The phonon energy and damping of the  $A_{1g}$  mode as function of T and h are calculated and compared for AgCrS<sub>2</sub>, AgCrO<sub>2</sub> and CuCrO<sub>2</sub>.

**Γ7.28.** I. N. Apostolova, A. T. Apostolov and J. M. Wesselinowa, Microscopic theory of the

### specific absorption rate for self-controlled magnetic hyperthermia, Journal of Magnetism and Magnetic Materials <u>522</u>, 167504 (2021).

ISSN 0304-8853, Q<sub>2</sub>, SJR 0,606, IF 3,097 doi: 10.1016/j.jmmm.2020.167504

#### Abstract:

Despite the efforts of many research teams, to optimize the process of thermal heating of magnetic nanoparticles interacting with an alternating magnetic field for self-controlled magnetic hyperthermia remains a challenge. Macroscopic models that quantify the process of heat generation could not combine the biocompatibility requirements of magnetic nanoparticles in human medicine on one hand with high values of specific absorption rate (SAR) on the other. For the first time, we propose a microscopic model using Kubo formalism, a modified Heisenberg Hamiltonian and the method of Green's functions for calculating the absorbed power (thermal energy absorbed by a magnetic nanoparticle per unit time in an alternating magnetic field). From the observed transverse magnetic susceptibility, elementary excitation energy, and damping is investigated the SAR as a function of the microscopic parameters of the systems: exchange interaction constants and single-ion magnetic anisotropy. The calculations are made for a magnetic complex heterogeneous nanoparticle consisting of core, shell, intermediate layer between them, and surface (the so called core/shell model). The proposed nanoparticle model allows for each region to define different exchange interaction and magnetic anisotropy constants as well as different magnetic configurations and thickness. The dependence of SAR on the microscopic parameters of the system is analyzed and qualitatively explained by the behavior of the elementary excitations (spin energy and damping). The results are in good qualitative agreement with the experimental data and show that using complex magnetic nanoparticles the heating properties for hyperthermia could be maximized.

**Γ7.29.** A. T. Apostolov, I. N. Apostolova and J. M. Wesselinowa, Magnetic and electric properties of multiferroic LiFeP<sub>2</sub>O<sub>7</sub>. Comparison with LiCrP<sub>2</sub>O<sub>7</sub>, Modern Physics Letters B <u>33(09)</u>, 2150158 (2021).

ISSN (print) 0217-9849, ISSN (online) 1793-6640, Q<sub>3</sub>, SJR 0,343, IF 1,948 doi: 10.1142/S021798492150158X

#### Abstract:

The temperature and magnetic field dependence of the magnetic and electric properties of LiFeP<sub>2</sub>O<sub>7</sub> (LFPO) and LiCrP<sub>2</sub>O<sub>7</sub> (LCPO) are studied using a microscopic model and the Green's function technique. We have shown that LFPO is antiferromagnetic, but shows a weak ferromagnetism along the *b* axis which originates from the canted antiferromagnetic order. For LCPO, such a ferromagnetic order along the *b* axis is not observed. In the temperature dependence of the electrical polarization  $P_b(T)$  along the *b* axis there is a kink at  $T_N = 22$  K which is an indirect evidence for the intrinsic magnetoelectric effect in LFPO. Applying an external magnetic field  $H_b$ , the polarization  $P_b$  increases, stronger for small temperatures and the kink at  $T_N$  disappears. For LCPO, we do not obtain a kink at  $T_N = 6$  K. LCPO is polar, but not ferroelectric. We can conclude that the missing magnetoelectric properties in LCPO could be due to the differences in the magnetic orders between LFPO and LCPO.

# Γ7.30. I. N. Apostolova, A. T. Apostolov and J. M. Wesselinowa, Magnetic, dielectric and optical properties of Al, Mg, Co and Zn ion doped CuCrO<sub>2</sub>, Europhysics Letters <u>133</u>, 47003 (2021). ISSN (print) 0295-5075, ISSN (online) 1286-4854, Q<sub>2</sub>, SJR 0,525, IF 1,958 doi: 10.1209/0295-5075/133/47003

#### Abstract:

The effects of Al, Mg, Co and Zn ion doping on different properties of multiferroic CuCrO<sub>2</sub> are studied using a microscopic model and the Green's function technique. The temperature dependence of the dielectric constant  $\epsilon'_{ab}$  shows a kink near  $T_N$ . For Al ion doping  $\epsilon'_{ab}$  decreases, for Co it increases, whereas for Mg it has a maximum for  $x \sim 0.1$ .  $\epsilon'_{ab}$  decreases with increasing magnetic field  $h_{ab}$ . The magnetization M is reduced with enhancing the Al and Zn doping concentration, whereas by Mg doping M shows a maximum at  $x \sim 0.1$ . The band gap  $E_g$  increases weakly for Zn doping. It decreases strongly with increasing Co and slightly with increasing Mg doping, which is in good quantitative agreement with the experimental data.

**F7.31. I. N. Apostolova, A. T. Apostolov and J. M. Wesselinowa, Multiferroic and phonon** properties at the phase transition of S = 1/2 chain cuprates NaCu<sub>2</sub>O<sub>2</sub>. Comparison with LiCu<sub>2</sub>O<sub>2</sub>, Phase Transitions <u>94</u>(6-8), 527-535 (2021).

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ISSN (print) 1029-0338, ISSN (online) 0141-1594, Q<sub>3</sub>, SJR 0,282, IF 1,529
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doi: 10.1080/01411594.2021.1945059

#### Abstract:

The multiferroic properties of NaCu<sub>2</sub>O<sub>2</sub> (NCO) around the phase transition temperature  $T_N$  are studied theoretically. The total polarization P is zero without magnetic field h due to the antiferroelectric state induced by the alternate stacking of CuO<sub>2</sub> layer with opposite spin vector chirality. Applying h Pincreases, goes through a maximum and vanishes at  $T_N$ . The magnetic field dependence of P(h) is an evidence that NCO is multiferroic. For h = 0 there is no anomaly in the dielectric constant  $\epsilon'$  at  $T_N$ which is an evidence for the antiferroelectric behavior of the compound. It is observed that P(h) and  $\epsilon'(h)$  in NCO is quite different compared to that of LiCu<sub>2</sub>O<sub>2</sub>. Around the Neel temperature  $T_N$  we observe in NCO an anomaly in the specific heat and the phonon energy due to strong anharmonic spinphonon interaction. This kink disappears by applying an external magnetic field h.

Γ7.32. A. T. Apostolov, I. N. Apostolova, J. M. Wesselinowa, Multiferroic properties of the antiferroelectric-antiferromagnetic Cu<sub>9</sub>O<sub>2</sub>(SeO<sub>3</sub>)<sub>4</sub>Cl6, Physics Letters A <u>407</u>, 127480 (2021).
ISSN (Print) 0375-9601, ISSN (Online) 1873-2429, Q<sub>2</sub>, SJR 0,531, IF 2,707 doi: 10.1016/j.physleta.2021.127480

#### Abstract:

The recently experimentally observed multiferroic properties of the antiferroelectric-antiferromagnetic -  $Cu_9O_2(SeO_3)_4C_{16}$  are studied using a microscopic model and a Green's function technique. The sublattice polarization increases with decreasing temperature and increasing magnetic field *h*. For the total polarization which is zero without electric field *E* is observed a double hysteresis loop. The dielectric constant shows two anomalies at the two transition temperatures  $T_N$  and  $T_E$ . The magnetoelectric ratio increases with increasing magnetic field below  $T_N$ . It is shown that a large magnetoelectric coupling g (E = 0) or a strong external electric field E (g = const) induces a weak ferromagnetism in this compound. In analogy g (h = 0) or an external magnetic field h (g = const) can lead to a weak ferroelectricity.

**F7.33.** I. N. Apostolova, A. T. Apostolov, S. Trimper and J. M. Wesselinowa, Dielectric properties of relaxor CuCrO<sub>2</sub> at room temperature, Physica Status Solidi B: Basic Solid State Physics 258(10), 2100136 (2021).

ISSN (Print) 0370-1972, ISSN (Online) 1521-3951, Q<sub>3</sub>, SJR 0,414, IF 1,782 doi: 10.1002/pssb.202100136

#### Abstract:

The dielectric properties of CuCrO<sub>2</sub> bulk and thin films are studied by evaluating the complex dielectric function  $\varepsilon$ . In addition to the small peak near the Néel temperature  $T_N$ , a secondary broad peak is found at high temperatures around  $T_m = 450 \text{ K} \gg T_N$ . As a feature of relaxor ferroelectrics, the maximum temperature  $T_m$  increases with increasing frequency. The real part of  $\varepsilon$  decreases with increasing magnetic field *h* and the peak at  $T_N$  vanishes. The secondary peak becomes smaller and is broadened with increasing magnetic field.  $\varepsilon$  increases with increasing film thickness. Near  $T_m$ , the dielectric function offers a critical behavior expressed by an exponent  $\gamma = 1.74$ . Using scaling arguments, critical exponents  $\beta = 0.13$  and  $\delta = 13.38$  are deduced. The exponents depend on the film thickness. While  $\beta$  increases, the exponent  $\gamma$  is reduced with increasing film thickness.

Γ7.34. A. T. Apostolov, I. N. Apostolova, J. M. Wesselinowa, Multiferroic and phonon properties near the phase transitions of pure and ion doped  $Ca_3Mn_2O_7$ , Phase Transitions <u>94</u>(10), 705-714 (2021).

### ISSN (print) 1029-0338, ISSN (online) 0141-1594, Q<sub>3</sub>, SJR 0,282, IF 1,529 doi: 10.1080/01411594.2021.1966003

#### Abstract:

The magnetic, dielectric and phonon properties of Ca<sub>3</sub>Mn<sub>2</sub>O<sub>7</sub> are investigated using a microscopic model and the Green's function technique. Electrically induced decrease of the magnetization M is observed which is an indirect evidence that Ca<sub>3</sub>Mn<sub>2</sub>O<sub>7</sub> is a multiferroic material. The dielectric function  $\epsilon'$  has an anomaly at the Neel temperature  $T_N$  and a broad peak at the Curie temperature  $T_C$ .  $\epsilon'$  increases with increasing magnetic field. M and  $T_N$  are enhanced by Li ion doping, whereas reduced by Ti ion doping due to different strain caused by the doped ions which changes the exchange interaction constants.  $T_C$  increases with increasing Ti concentration. The temperature and magnetic field dependence of the phonon energy and damping for the A<sub>1</sub> mode  $\omega_0 = 624$  cm<sup>-1</sup> are studied. Both show a kink at  $T_N$  due to the strong spin–phonon interaction. The kink disappears applying a magnetic field.

### Γ7.35. Iliana Apostolova, Angel Apostolov, J. M. Wesselinowa, Phonon and optical properties of transition metal and rare earth ion doped BaTiO<sub>3</sub>, Journal of Applied Physics <u>130</u>(17), 175103 (2021).

ISSN (print) 1089-7550, ISSN (online) 0021-8979, Q<sub>2</sub>, SJR 0,668, IF 2,877 doi: 10.1063/5.0069464

#### Abstract:

We have calculated the phonon energy and damping of  $\omega_0 = 264 \text{ cm}^{-1}$  in Fe, Mn, and Dy doped BaTiO<sub>3</sub> using a microscopic model. By doping with Fe ions, the phonon energy  $\omega$  and damping  $\gamma$  show anomalies at the two phase transition temperatures.  $\omega$  increases whereas  $\gamma$  decreases with the increase in the magnetic field and the kink at  $T_C^{fm}$  vanishes.  $\omega$  and  $T_C^{fe}$  decrease or increase with the increase in Mn or Fe dopants, respectively.  $T_C^{fe}$  and  $\omega$  of  $\omega_0 = 718 \text{ cm}^{-1}$  decrease with the increase in Dy ion doping on the Ba site.  $\gamma$  is enhanced for all three ions. The changes in the phonon properties by ion doping are due to the different strain caused by the different ionic radii of the host and doping ions. The effects of Fe, Mn, and Sm doping on the bandgap energy are also discussed.

### Γ7.36. A. T. Apostolov, I. N. Apostolova, J. M. Wesselinowa, Application of ion doped $Y_3Fe_5O_{12}$ nanoparticles for self-controlling magnetic hyperthermia, Physica Status Solidi B: Basic Solid State Physics <u>259</u>(3), 2100545 (2022). ISSN (Print) 0370-1972, ISSN (Online) 1521-3951, Q<sub>3</sub>, SJR 0,401, IF 1,6

#### doi: 10.1002/pssb.202100545

#### Abstract:

Herein, doped yttrium garnet (YIG) nanoparticles (NPs)  $Y_3[Fe_{2-y}M_y]_a(Fe_{3-z}M_z)_dO_{12}$  (M = Al, Ga, Sc are nonmagnetic ions) are studied, appropriate for self-controlled magnetic hyperthermia (SCMH) for in vivo and in vitro applications. A microscopic model (modified Heisenberg Hamiltonian) and the Green's function technique are used to investigate the temperature, doping, and size dependence of magnetic phase transition, saturation magnetization, the coercivity, and the specific absorption rate coefficient to fulfill the conditions for magnetic hyperthermia. A set of mixed yttrium garnet magnetic NPs is found, which are suitable for applications in medicine for cancer therapy. There are two Sc-doped YIG NPs which are the best candidates for SCMH with x = 1.08, d = 27.5 nm, and SAR<sub>max</sub> = 13.52 W g<sup>-1</sup>, as well as x = 1.10, d = 29.7 nm, and SAR<sub>max</sub> = 15.44 W g<sup>-1</sup> for which the conditions for biocompatibility and maximization of SAR are fulfilled simultaneously. Moreover, also Al- and Ga-doped YIG NPs are found that can be applied for magnetic hyperthermia but with smaller SAR effectivity.

## **Γ7.37.** A. T. Apostolov, I. N. Apostolova, J. M. Wesselinowa, Magnetic, electric and optical properties of ion doped CuCr<sub>2</sub>O<sub>4</sub> nanoparticles, Magnetochemistry <u>8</u>, 122 (2022). ISSN 2312-7481, Q<sub>2</sub>, SJR 0,42, IF 2,7 doi: 10.3390/magnetochemistry8100122

Abstract:

The magnetic, electric and optical properties of pure and ion doped CuCr<sub>2</sub>O<sub>4</sub> - bulk and nanoparticles

are investigated theoretically. The magnetization  $M_S$  and the band gap  $E_g$  decrease with increasing particle size. By Co ion doping  $M_S$  and the polarization P show a maximum whereas by Pr ion doping they decrease with increasing the doping concentration. The dielectric constant decreases with enhancing Pr dopants. It is shown that the difference between the doping and host ions radii leads to appearing of a compressive or tensile strain and to different exchange interaction constants in the doped state.  $E_g$  decreases by Co doping, whereas it increases by Pr doping.

#### **Γ7.38. I. N. Apostolova, A. T. Apostolov, J. M. Wesselinowa, Size and ion doping effects on** magnetic, optical and phonon properties of CuAlO<sub>2</sub>, Magnetochemistry <u>8</u>, 169 (2022). ISSN 2312-7481, Q<sub>2</sub>, SJR 0,42, IF 2,7 doi: 10.3390/magnetochemistry8120169

#### Abstract:

The magnetic, optical, and phonon properties of ion-doped CuAlO<sub>2</sub> nanoparticles on the Cu or Al site are theoretically investigated. The room temperature ferromagnetism in CuAlO<sub>2</sub> nanoparticles can be due to the surface, size, and doping effects. The magnetization increases with the decreasing nanoparticle size. The different radii of the transition metal ion and the host Cu ion lead to compressive strain, to the enhancment of the exchange interaction constants, and to increased magnetization  $M_S$  and Curie temperature  $T_C$ . By substitution with Mn or Cr on the Al site, tensile strain, a decrease in  $M_S$ , and an increase in dopants are observed. The size and ion-doping influence on the band-gap energy is also discussed. The phonon energy  $\omega$  decreases, whereas the phonon damping  $\gamma$  increases with increasing temperature and decreasing NP size. They show a kink around  $T_C \sim 400$  K. The behavior of  $\omega$  and  $\gamma$  for different ion dopings is observed.

# **Γ7.39.** Iliana Apostolova, Angel Apostolov and Julia Wesselinowa, Magnetic, phonon and optical properties of transition metal and rare earth ion doped ZnS nanoparticles, Nanomaterials <u>13</u>, 79 (2023). ISSN 2079-4991, Q<sub>1</sub>, SJR 0,81, IF 5,3(2022) doi: 10.3390/nano13010079

#### Abstract:

The surface, size and ion doping effects on the magnetic, phonon and optical properties of ZnS nanoparticles are studied based on the s-d model including spin-phonon and Coulomb interaction, and using a Green's function theory. The changes of the properties are explained on a microscopic level, due to the different radii between the doping and host ions, which cause different strains -compressive or tensile, and change the exchange interaction constants in our model. The magnetization increases with increasing small transition metal (TM) and rare earth (RE) doping concentration. For larger TM dopants the magnetization decreases. The phonon energies increase with increasing TM, whereas they decrease by RE ions. The phonon damping increases for all doping ions. The changes of the band gap energy with different ion doping concentration is also studied. Band gap changes in doped semiconductors could be due as a result of exchange, s-d, Coulomb and electron-phonon interactions. We have tried to clarify the discrepancies which are reported in the literature in the magnetization and the band gap energy.

#### **Γ7.40.** Iliana Apostolova, Angel Apostolov and Julia Wesselinowa, Band Gap Tuning in Transition Metal and Rare-Earth-Ion-Doped TiO<sub>2</sub>, CeO<sub>2</sub>, and SnO<sub>2</sub> Nanoparticles, Nanomaterials <u>13</u>, 145 (2023). ISSN 2079-4991, Q<sub>1</sub>, SJR 0,81, IF 5,3(2022) doi: 10.3390/nano13010145

#### Abstract:

The energy gap  $E_g$  between the valence and conduction bands is a key characteristic of semiconductors. Semiconductors, such as TiO<sub>2</sub>, SnO<sub>2</sub>, and CeO<sub>2</sub> have a relatively wide band gap  $E_g$  that only allows the material to absorb UV light. Using the s-d microscopic model and the Green's function method, we have shown two possibilities to reduce the band-gap energy  $E_g$  -reducing the NP size and/or ion doping with transition metals (Co, Fe, Mn, and Cu) or rare earth (Sm, Tb, and Er) ions. Different strains appear that lead to changes in the exchange-interaction constants, and thus to a decrease in  $E_g$ . Moreover, the importance of the s-d interaction, which causes room-temperature ferromagnetism and band-gap energy tuning in dilute magnetic semiconductors, is shown. We tried to clarify some discrepancies in the experimental data.

# **Γ7.41.** A. T. Apostolov, I. N. Apostolova, J. M. Wesselinowa, Differences between the multiferroic properties of hexagonal and orthorhombic ion doped YFeO<sub>3</sub> nanoparticles, International Journal of Modern Physics B <u>37</u>(21), 2350201 (13 pages) (2023). ISSN (Print) 0217-9792, ISSN (Online) 1793-6578, Q<sub>3</sub>, SJR 0,27, IF 1,7(2022) doi: 10.1142/S0217979223502016

#### Abstract:

The multiferroic properties of ion-doped hexagonal and orthorhombic YFeO<sub>3</sub> (YFO) nanoparticles (NPs) are studied theoretically. The magnetization  $M_s$  in h-YFO NPs increases, whereas for o-YFO NPs it decreases with decreasing NP size. In the dielectric constant (DC) both h- and o-YFO have a peak around  $T_{C1}$ ~450 and 460 K, respectively, but only in h-YFO an anomaly appears at  $T_{C2}$ ~300 K in the DC and the polarization which could be connected with a possible P6<sub>3mc</sub>–P6<sub>3cm</sub> phase transition. The polarization in pure and Bi-doped o-YFO NPs increases with increasing magnetic field.  $M_s(x)$  is studied by doping of a o-YFO NP with Ti<sup>4+</sup> ions at the octahedral Fe<sup>3+</sup> sites.  $M_s(T)$  in undoped YFO shows a small kink at  $T_{C1}$ ~450 K, whereas in the doped YFO it shows at ~480 K. By different ion doping on the Y or Fe sites in YFO there is a transformation from the h- to the o-phase or vice versa. In Mn-doped o-YFO a spin-reorientation transition appears. The bandgap of h-YFO is smaller compared to that of o-YFO.

# **Γ7.42.** Iliana Apostolova, Angel Apostolov and Julia Wesselinowa, Magnetic, optical and phonon properties of ion doped MgO nanoparticles. Application for magnetic hyperthermia, Materials <u>16</u>, 2353 (2023). ISSN 19961944, Q<sub>2</sub>, SJR 0,56, IF 3,4(2022) doi: 10.3390/ma16062353

#### Abstract:

The influence of size and doping effects on the magnetization M, phonon  $\omega$  and band gap energy  $E_g$  of MgO nanoparticles is studied using a microscopic model. The room-temperature ferromagnetism is due to surface or/and doping effects in MgO nanoparticles (NPs). The influence of the spin-phonon interaction is discussed. M increases with decreasing NP size. M and  $E_g$  can increase or decrease by different ion doping (Co, Al, La, Fe) due to the different strain that appears. It changes the lattice parameters and the exchange interaction constants. We found that MgO NP with size of 20 nm and Feor Co-doping concentration x = 0.1 and x = 0.2, respectively, have a Curie temperature  $T_C = 315$  K, i.e., they are appropriate for application in magnetic hyperthermia, they satisfy the conditions for that. The energy of the phonon mode  $\omega = 448$  cm<sup>-1</sup> increases with decreasing NP size. It increases with increasing Co and Fe, or decreases with Sr ion doping.

### Γ7.43. Iliana Apostolova, Angel Apostolov and Julia Wesselinowa, Comparison of the multiferroic properties of ion doped hexagonal LuFeO<sub>3</sub> and LaFeO<sub>3</sub> Physica Status Solidi B: Basic Solid State Physics <u>260</u>(7), 2300077 (2023).

ISSN (Print) 0370-1972, ISSN (Online) 1521-3951, Q<sub>3</sub>, SJR 0,401, IF 1,6(2022) doi: 10.1002/pssb. 202300077

#### Abstract:

Using a microscopic model, the magnetic and electric properties of pure and ion-doped (on the Lu or Fe sites) hexagonal LuFeO<sub>3</sub> (LuFO) are studied and compared with the properties of ion-doped LaFeO<sub>3</sub> (LaFO). The magnetization increases by Sr and Sc doping which is caused by the strain and the changes of the exchange interaction constants at the doped states. It is observed that by Sm doping of LuFO the polarization decreases, whereas by Sm doping of LaFO, the polarization increases with increasing Sm concentration. By Ir or Co ion doping on the Fe site, the magnetization and the phonon energy increase whereas the bandgap energy decreases. By doping on the Fe sites with the same ion, for example, Sc, there are no differences between LuFO and LaFO. A good agreement with the experimental data is observed. The doping effects can be used for different applications.

## **Γ7.44.** Iliana Apostolova, Angel Apostolov and Julia Wesselinowa, Band gap energy of ion doped multiferroic NaFeO<sub>2</sub> nanoparticles, Physica Status Solidi (RRL) - Rapid Research Letters 2300159 (2023).

ISSN (Print) 1862-6254, ISSN (Online), 1862-6270, Q<sub>2</sub>, SJR 0,73, IF 2,8(2022) doi: 10.1002/pssr.202300159

#### Abstract:

The band gap energy  $E_g$  of orthorhombic  $\beta$ - and hexagonal  $\alpha$ -NaFeO<sub>2</sub> -bulk and nanoparticles is investigated for the first time based on a microscopic model combined with Green's function theory.  $E_g$ increases with decreasing nanoparticles size and is shape-dependent. The competition between Coulomb and electron-phonon interactions is demonstrated. Moreover,  $E_g$  decreases with increasing Ge and Si doping concentration or increases by Mn, Cr, and Ni ion doping due to different radii of the doping and the host Fe ions, leading to varying strains. The substitution for Na ion by K or Li(Cu) ions can cause both enhancing or reducing of  $E_g$ . Thus, the band gap energy can be regulated by nanoparticles size, ion doping, electron-phonon, and Coulomb interactions.

# **Γ7.45.** Iliana Naumova Apostolova, Angel Todorov Apostolov, Julia Mihailova Wesselinowa, Magnetoelectric coupling effects in Tb doped BiFeO<sub>3</sub> nanoparticles, Magnetochemistry <u>9</u>, 142 (2023). ISSN 2312-7481, Q<sub>2</sub>, SJR 0,42, IF 2,7(2022) doi: 10.3390/magnetochemistry9060142

#### Abstract:

The magnetic, electric, and optical properties in Tb-doped BiFeO<sub>3</sub> nanoparticles as functions of size and doping concentrations were investigated using a microscopic model, taking into account both linear and quadratic magnetoelectric (ME) coupling. We observed improved multiferroic properties and bandgap tuning. The magnetization and polarization increased with the decreased nanoparticle size and increased Tb-doping substitution x. The Neel temperature remained nearly unchanged whereas the Curie temperature was reduced with the increased x. There was doping-induced ME coupling. The dielectric constant is discussed as a function of the size, doping, and the magnetic field. The band gap decreased with the decreased size or increased Tb dopants due to competing effects of the compressive strain, oxygen defects on the surface, and Coulomb interactions. Increasing the Tb dopants and decreasing the nanoparticle size improved the ME effect.

## **Γ7.46.** Iliana Apostolova, Angel Apostolov and Julia Wesselinowa, Size and doping effects on the magnetic and electric properties of Bi<sub>2</sub>Fe<sub>4</sub>O<sub>9</sub> nanoparticles, European Physical Journal B <u>96</u>, Article number: 77 (2023).

ISSN (Print) 1434-6028, ISSN (Online) 1434-6036, Q<sub>3</sub>, SJR 0,379, IF 1,6(2022) doi: 10.1140/epjb/s10051-023-00550-x

#### Abstract:

In the present paper we propose a microscopic model to study the multiferroic properties of Bi<sub>2</sub>Fe<sub>4</sub>O<sub>9</sub> nanoparticles. The spontaneous magnetization  $M_S$  increases with decreasing nanoparticle size.  $M_S$  is shape dependent. It is larger for cylindrical than for spherical nanoparticles.  $M_S$  increases with increasing Co and Ho concentration, whereas by Mn doping it decreases. These tunable magnetic properties can be widely applied in spintronics. The polarization  $P_S$  increases also with decreasing nanoparticle size. Mn ion doping leads to increase of  $P_S$ , the phase transition temperature  $T_C$  and the dielectric constant and so to enhanced electric and dielectric properties of Bi<sub>2</sub>Fe<sub>4</sub>O<sub>9</sub> nanoparticles. Applying an external magnetic field  $P_S$  is enhanced, which is indirect evidence for a strong magnetoelectric coupling. The specific heat  $C_P$  shows an anomaly at the Neel temperature  $T_N$  which vanishes by applying an external magnetic field. The band gap energy  $E_g$  decreases with increasing Ti, Co and Ho dopants whereas by Mn doping  $E_g$  increases.

**Γ7.47.** Iliana Apostolova, Angel Apostolov and Julia Wesselinowa, Magnetic properties of Gd-Doped Fe<sub>3</sub>O<sub>4</sub> nanoparticles, Applied Sciences <u>13</u>(11), 6411 (2023).

#### ISSN 2076-3417, Q<sub>2</sub>, SJR 0,49, IF 2,7(2022) doi: 10.3390/app13116411

#### Abstract:

The magnetic properties of pure and rare earth ion-doped  $Fe_3O_4$  nanoparticles are investigated using a microscopic model and the Green's function theory. The magnetization  $M_S$  and Curie temperature  $T_C$  are calculated depending on size, temperature and Gd doping concentration.  $M_S$  and  $T_C$  decrease with decreasing nanoparticle size and with increasing the doping concentration. The band gap energy increases with decreasing size and Gd dopants. The obtained results are in good agreement with the experimental data.

### E19. A published university textbook or a textbook that is used by school establishments.

E19.1. И. Апостолова, А. Апостолов, Физика с биофизика, Издателство "Авангард прима", ISBN 978-619-160-677-1, 323 стр., София (2016).

E19.1. I. Apostolova, A. Apostolov, Physics with biophysics, Avangard Prima Publishing House, ISBN 978-619-160-677-1, 323 pages, Sofia (2016).

#### Abstract:

The textbook was written according to the lecture course "Physics with the basics of biophysics" for the students of the Veterinary Medicine specialty at LTU. The unification in one course of parts of general physics and biophysics made it necessary to select such physics topics that are closely related to medicine, as well as to consider only parts of biophysics (molecular biophysics and biophysics of the cell). The study material is systematized in eight parts: Acoustics and bioacoustics, Molecular physics and thermodynamics of biological systems, Electricity and magnetism, Optics, Biological and artificial membranes, Transport of substances through biomembranes, Electrical properties of cells and tissues and Biopotentials. In the first part of the textbook, more traditional physics topics are presented, and at the end of each of them, their relationship with the processes taking place in living organisms is shown. Basic imaging methods - ultrasound, thermography and magnetic resonance imaging have been reviewed. The second part of the textbook is entirely biophysical, purposefully exploring links with physiology, biochemistry and molecular biology.

### E19.2. И. Апостолова, Физика с биофизика за еколози, Издателство "Авангард прима", ISBN 978-619-239-896-5, 373 стр., София (2023).

E19.2. I. Apostolova, Physics with biophysics for ecologists, Avangard Prima Publishing House, ISBN 978-619-239-896-5, 373 pages, Sofia (2023).

#### Abstract:

The textbook was written according to the lecture course "Physics with Biophysics" for the students of the Ecology and Environmental Protection at LTU. It examines basic ideas and methods of physics and biophysics, paying attention to the physical side of the phenomena and regularities related to the protection of nature and climate. The study material is systematized in six parts: Types of movements; Mechanical vibrations and waves; Types of interactions; Electric and magnetic field; Thermodynamics and molecular physics; Energy conversion in biological systems; Cell membrane and substance transport; Electrical and magnetic properties of substances; Electrical properties of tissues and Electromagnetic and corpuscular radiations and their interaction with substances. The topics explored in the textbook are relevant to the work and further education of future ecologists and help them develop accurate thinking and precision and gain insight into the essence of natural phenomenon. Topics related to aeroions, their biological action and the consequences of ion balance disruption, the greenhouse effect and climate change, the ozone hole and its impact on living organisms, leading to the disruption of the balance in ecosystem are discussed from a physical point of view. Particular attention is paid to the natural and man-made sources of ionizing corpuscular and photon radiation and the principles on which protection against them is based. The biological action of ionizing radiations and the deterministic and stochastic damage caused by them, doses and dose loading are examined. Basic physical methods for qualitative and quantitative determination of the chemical composition of substances and the possibility of observing various biological objects are briefly discussed.

E20. A published university textbook or a textbook that is used by school establishments.

E20.1. И. Апостолова, Тестове по Физика и Физика с биофизика за студентите от Лесотехнически университет, Издателство "Авангард прима", ISBN 978-619-239-712-8, 144 стр., София, (2022).

E20.1. I. Apostolova, Tests in Physics and Physics with Biophysics for Forestry University Students, Avangard Prima Publishing House, ISBN 978-619-239-712-8, 144 pages, Sofia, (2022).

#### Abstract:

The exam preparation book is intended for all LTU students studying the disciplines "Physics" - Forestry, Wood and Furniture Technology, Engineering Design, Computer Technologies in the Furniture Industry and "Physics with Biophysics" - Veterinary Medicine, Ecology and Environmental Protection, Agronomy and Plant Protection. Its purpose is to help students absorb more knowledge during the academic semester, and not just rely on the session. This can be done through appropriate and objective in-semester assessments consisting of laboratory exercises, the results of which are weighted appropriately in the formation of the final grade of the "Physics" and "Physics with Biophysics" exams. The tests were developed on the basis of the "Manual for Laboratory Exercises in Physics and Biophysics" of LTU. Each test contains multiple open and closed questions. The tool can be used both for self-training by the students and by other physicist colleagues for in-semester assessments.

January 2024

Prepared by:

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