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Editorial

Magnetic, Dielectric, Electrical, Optical and Thermal Properties of Crystalline Materials

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This Special Issue entitled "Magnetic, Dielectric, Electrical, Optical and Thermal Properties of Crystalline Materials" is devoted to a general overview of the subject of crystalline materials and may extend to the nanocrystalline field. The articles published within it relate to the composition selection, the optimization of processing conditions and the structural and functional response. Thus, this Special Issue includes synthesis, characterization and applications studies. The properties, the structure and the mechanical, magnetic, dielectric, optical and thermal properties of these crystalline materials are the focus of interest [1–4].

As remarked in the Special Issue information, the keywords of the fifteen manuscripts published are a good indicator of the main fields of interest. The production techniques employed include rapid solidification, sol-gel, mechanical alloying, co-precipitation, liquid-phase epitaxy, click chemistry, and deposition techniques. The materials used are Heusler alloys, tungsten-based materials, copper–tin alloys, manganese–nickel alloys, gallium-based magnetic semiconductors, ferrimagnetic iron garnet films, cadmium base spinel, aluminum base alloys, oxychalcogenide compounds, porphyrin complexes, Janus bidimensional monolayers or cross-linked sodium alginate and polyacrylic acid biopolymers, and ferrite oxides. The structural information provided, based on the specific crystalline structures, includes crystallographic defects and solid-state structural transformations, such as the martensitic transformation and magnetic transformations, as well as ferromagnetic to paramagnetic transition. The mechanical properties analyzed include the elasticity, the strain, the creep mechanism, and the strengthening behavior. The studies of the electrical and dielectric properties are based in electrical conductivity or resistivity analysis, the electronic structure of the materials with ab initio theoretical studies, the study of the transport coefficients, orbital coupling, the semiconductor or piezoelectric behavior, and the study of the mechanisms of conduction. Magnetic analysis permits the determination of the ferromagnetic, ferrimagnetic, paramagnetic, or superparamagnetic behavior. Thermal analysis (characteristic temperatures, thermal treatments) is sometimes related to thermodynamics or kinetics, with parameters such as the activation energy. Optical analysis is linked to UV absorption, photoelectronic and photovoltaic analysis. Specific applications include dye degradation and antimicrobial, antioxidant, and anticancer activity.

Two articles are devoted to applications of Heusler alloys. Rekik et al. produce and analyze the structure and the thermal and kinetic behavior of the martensitic transformation of a Mn rich Mn–Ni–Sn compound. The Heusler alloys of the Mn–Ni–Sn family are candidates for implementation in magnetic refrigeration devices due to their magnetocaloric effect. Thus, the transition temperature control and the activation energy of the transformation are of interest. Hzzazi et al. produce quaternary Co–M–Rh–Si (M = Cr, Mn) Heusler alloys. These materials are candidates for spintronic and thermoelectric applications due to their high transport coefficients (electrical conductivity, Seebek coefficient) and can provoke highly spin-polarized currents. The density functional theory (DFT) determines the to-

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tal energy, phonon, and elastic behavior and complements the magnetic and functional response analysis.

One of the main fields of interest of crystalline materials is their environmental applications [5]. Two articles introduce an environmental application, namely the degradation of dyes. Nasri et al. synthesize porphyrin complexes. In this case, the degradation mechanism is a catalytic effect. The current–voltage response and the impedance spectroscopy measurements confirm that these complexes are candidates for optoelectronic applications such as in photovoltaic devices. Ben Mbarek et al. produce a binary alloy Mn–Al produced by mechanical alloying which provokes the degradation of azo dyes by means of a redox mechanism. UV absorption and infrared spectroscopy measurements confirm the discoloration of the dissolutions.

There are some studies based on the density functional theory [6]. This is an optimal approach for theoretical calculations of the electron density and energy distribution, the spin bad structures, the spin channels, and the spin-polarized density. It permits us to understand the interactions between electrons and ions. Zhang et al. apply DFT (considering the first-principles plane-wave pseudopotential method) to understand the effect of tin content in the structure, the elastic response, and the electronic properties of binary Cu–Sn alloys. The best content regarding structural stability is 3.125 at. % of Sn, whereas the best content for plasticity and elastic anisotropy is 6.25 at. % Sn. Tian et al. apply the DFT generalized gradient approximation and the Perdew–Nurke–Erzerhof formalism in diluted magnetic semiconductors (Ga–N-based ferromagnetic monolayers) to calculate the electronic and magnetic properties. Mallah et al. also produce, characterize, and analyze DFT monolayers. In this study, there are bidimensional Janus (two faces with two different local environments) monolayers. These monolayers consist of A_2XX', Si_2XX' and A_2PAs. These materials are candidates for application in piezoelectric nanodevices. The best results are observed for the materials containing chalcogenide atoms. In a second work, the same research team use the same methods to calculate the band structures and the density of states for several oxychalcogenides, including $A_2O_2B_2Se_3$ (A = Sr, Ba; B = Bi, Sb) compounds, and the optical and thermodynamic properties are analyzed. The reflectivity spectra confirm that these oxychalcogenides are optimal candidates for optical applications. Regarding mechanical behavior, some compounds are ductile, whereas $Ba_2O_2Sb_2Se_3$ is brittle.

Some articles characterize metallic alloys and compounds [7]. Chen et al. produce a cast heat-resistant aluminum alloy (Al–Si–Cu–Ni–Mg) by annealing the master alloy produced in an electric-smelling furnace. It is well known that the thermal treatment conditions (temperature, time, pressure, atmosphere) influence the microstructure and the mechanical response (tensile strength, elongation, creep). The authors analyze the main creep mechanism at low temperatures and low stress and detect that is a grain-boundary creep. Ferromagnetic rare-earth (gallium and gadolinium) iron garnet films were prepared via liquid-phase epitaxy. The authors analyze the structure and the magnetization near the compensation temperature, discovering the suppression effect of the non-colinear phase. The compensation temperature definition is as follows: the temperature at which the magnetizations of oppositely directed magnetic sub-lattices fully compensate one other. The authors used a magneto-optic approach to build the temperature–magnetic field (T-H) diagrams of the magnetic states in two- and three sub-lattice ferromagnetic structures.

Regarding properties, one article demonstrates the applicability of several cross-linked sodium alginate and polyacrylic acid biopolymers based on nanoscale natural polysacaccharides. This is a complex procedure, and nano-sized metallic polymers are prepared from the biopolymers. There are environmental and health applications due to the antimicrobial and anticancer activity (drug delivery) and the antioxidant and non-toxic (biocompatibility, biodegradability) behavior.

A large number of articles are devoted to oxides [8]. Mahmood et al. synthesized ZnO nanotube-based magnetic semiconductors and analyzed the effect of the addition of cobalt and gadolinium on the structure and the dielectric and magnetic properties. Both additions improve the electrical conductivity and the ferromagnetic behavior (exception

Gd doping >3 at. %) due to the magnetic impurities replaced in the ZnO oxide. These materials are candidates for spintronic electronic charge, quantum Hall effect, or resistive switching devices. Alharbi et al. synthetize complex ferrites with spinel structures as nanoparticles. The compositions are $Cd_{0.5}Zn_{0.5}Fe_{2-x}Cr_xO_4$ ($0 \leq x \leq 2$). The vibrations of the metal–oxygen bonds in the spinel structure provoke the detection of two absorption bands in infrared spectroscopy analysis. The nanocrystalline size decreases as the content of Cr increases. These materials are potential candidates for electronics (power transformers) and telecommunications applications. Krimi et al. produce lithium–sodium–tungsten-based oxides and analyze the optical, dielectric, and electric properties. The influence of the partial substitution of lithium by sodium is checked. The addition of sodium favors the formation of an orthorhombic crystallographic structure. Likewise, the increase in the disorder and the charge number provokes an increase in the conductivity. The last referred article in this Special Issue corresponds to nickel–zinc ferrites produced by means of the sol-gel method by Mallah and coworkers. Complex hyperfine structures are detected due to the different atomic neighbors having different magnetic moments. Concerning the magnetic behavior, the ferromagnetism is influenced by the presence or absence of Ni^{2+} or Zn^{2+} ions in tetrahedral locations.

Finally, we express our thanks to all of the contributors to this Special Issue, all of the reviewers for their help in improving the quality and soundness of the manuscripts, and especially the MDPI staff. The editors hope that the articles presented in this Special Issue are of interest to researchers producing crystalline alloys and compounds with magnetic, dielectric, electrical, optical, and thermal properties.

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List of Contributions:

1. Rekik, H.; Hammami, B.; Khitouni, M.; Bachagha, T.; Suñol, J.-J.; Chemingui, M. Microstructure and Kinetics of Thermal Behavior of Martensitic Transformation in (Mn,Ni)Sn Heusler Alloy. *Crystals* **2022**, *12*, 1644. https://doi.org/10.3390/cryst12111644.
2. Hzzazi, A.; Alqurashi, H.; Andharia, E.; Hamad, B.; Manasreh, M.O. Theoretical Investigations of the Structural, Dynamical, Electronic, Magnetic, and Thermoelectric Properties of Co*M*RhSi (*M* = Cr, Mn) Quaternary Heusler Alloys. *Crystals* **2024**, *14*, 33. https://doi.org/10.3390/cryst14010033.
3. Nasri, S.; Guergueb, M.; Brahmi, J.; O. Al-Ghamdi, Y.; Loiseau, F.; Nasri, H. Synthesis of a Novel Zinc(II) Porphyrin Complex, Halide Ion Reception, Catalytic Degradation of Dyes, and Optoelectronic Application. *Crystals* **2023**, *13*, 238. https://doi.org/10.3390/cryst13020238.
4. Mbarek, W.B.; Al Harbi, M.; Hammami, B.; Khitouni, M.; Escoda, L.; Suñol, J.-J. Nanostructured Mn–Ni Powders Produced by High-Energy Ball-Milling for Water Decontamination from RB5 Dye. *Crystals* **2023**, *13*, 879. https://doi.org/10.3390/cryst13060879.
5. Zhang, L.; Li, Y.; Zhou, R.; Wang, X.; Wang, Q.; Xie, L.; Li, Z.; Xu, B. First-Principles Study of the Effect of Sn Content on the Structural, Elastic, and Electronic Properties of Cu–Sn Alloys. *Crystals* **2023**, *13*, 1532. https://doi.org/10.3390/cryst13111532.
6. Tian, S.; Zhang, L.; Liang, Y.; Xie, R.; Han, L.; Lan, S.; Lu, A.; Huang, Y.; Xing, H.; Chen, X. Room Temperature Ferromagnetic Properties of $Ga_{14}N_{16-n}Gd_2C_n$ Monolayers: A First Principle Study. *Crystals* **2023**, *13*, 531. https://doi.org/10.3390/cryst13030531.
7. Mallah, A.; Debbichi, M.; Dhaou, M.H.; Bellakhdhar, B. Structural, Mechanical, and Piezoelectric Properties of Janus Bidimensional Monolayers. *Crystals* **2023**, *13*, 126. https://doi.org/10.3390/cryst13010126.
8. Mallah, A.; Debbichi, M.; Dhaou, M.H.; Bellakhdhar, B. Structural, Mechanical, Electronic, Optical, and Thermodynamic Properties of New Oxychalcogenide $A_2O_2B_2Se_3$ (A = Sr, Ba; B = Bi, Sb) Compounds: A First-Principles Study. *Crystals* **2023**, *13*, 122. https://doi.org/10.3390/cryst13010122.

9. Chen, F.; Liu, C.; Zuo, L.; Wu, Z.; He, Y.; Dong, K.; Li, G.; He, W. Effect of Thermal Exposure on Mechanical Properties of Al-Si-Cu-Ni-Mg Aluminum Alloy. *Crystals* **2023**, *13*, 236. https://doi.org/10.3390/cryst13020236.
10. Suslov, D.A.; Vetoshko, P.M.; Mashirov, A.V.; Taskaev, S.V.; Polulyakh, S.N.; Berzhansky, V.N.; Shavrov, V.G. Non-Collinear Phase in Rare-Earth Iron Garnet Films near the Compensation Temperature. *Crystals* **2023**, *13*, 1297. https://doi.org/10.3390/cryst13091297.
11. Al-Fakeh, M.S.; Alazmi, M.S.; EL-Ghoul, Y. Preparation and Characterization of Nano-Sized Co(II), Cu(II), Mn(II) and Ni(II) Coordination PAA/Alginate Biopolymers and Study of Their Biological and Anticancer Performance. *Crystals* **2023**, *13*, 1148. https://doi.org/10.3390/cryst13071148.
12. Mahmood, M.A.; Khan, R.; Al Otaibi, S.; Althubeiti, K.; Abdullaev, S.S.; Rahman, N.; Sohail, M.; Iqbal, S. The Effect of Transition Metals Co-Doped ZnO Nanotubes Based-Diluted Magnetic Semiconductor for Spintronic Applications. *Crystals* **2023**, *13*, 984. https://doi.org/10.3390/cryst13070984.
13. Alharbi, R.K.; Kouki, N.; Mallah, A.; Beji, L.; Tar, H.; Algreiby, A.; Alnafisah, A.S.; Hcini, S. Processing and Investigation of $Cd_{0.5}Zn_{0.5}Fe_{2-x}Cr_xO_4$ ($0 \leq x \leq 2$) Spinel Nanoparticles. *Crystals* **2023**, *13*, 1121. https://doi.org/10.3390/cryst13071121.
14. Krimi, M.; Al-Harbi, M.H.; Alsulami, A.H.; Karoui, K.; Khitouni, M.; Ben Rhaiem, A. Optical, Dielectric, and Electrical Properties of Tungsten-Based Materials with the Formula $Li_{(2-x)}Na_xWO_4$ (x = 0, 0.5, and 1.5). *Crystals* **2023**, *13*, 1649. https://doi.org/10.3390/cryst13121649.
15. Mallah, A.; Al-Thuwayb, F.; Khitouni, M.; Alsawi, A.; Suñol, J.-J.; Greneche, J.-M.; Almoneef, M.M. Synthesis, Structural and Magnetic Characterization of Superparamagnetic $Ni_{0.3}Zn_{0.7}Cr_{2-x}Fe_xO_4$ Oxides Obtained by Sol-Gel Method. *Crystals* **2023**, *13*, 894. https://doi.org/10.3390/cryst13060894.

References

1. Radwan-Pragłowska, N.; Radwan-Pragłowska, J.; Łysiak, K.; Galek, T.; Janus, Ł.; Bogdał, D. Commercial-Scale Modification of NdFeB Magnets under Laser-Assisted Conditions. *Nanomaterials* **2024**, *14*, 431. [CrossRef]
2. Solozhenko, V.L.; Matar, S.F. High-Pressure Phases of Boron Pnictides BX (X = As, Sb, Bi) with Quartz Topology from First Principles. *Crystals* **2024**, *14*, 221. [CrossRef]
3. Hossen, M.F.; Shendokar, S.; Aravamudhan, S. Defects and Defect Engineering of Two-Dimensional Transition Metal Dichalcogenide (2D TMDC) Materials. *Nanomaterials* **2024**, *14*, 410. [CrossRef]
4. Puente-Córdova, J.G.; Luna-Martínez, J.F.; Mohamed-Noriega, N.; Miranda-Valdez, I.Y. Electrical Conduction Mechanisms in Ethyl Cellulose Films under DC and AC Electric Fields. *Polymers* **2024**, *16*, 628. [CrossRef]
5. Al-Kadhi, N.S.; Al-Senani, G.M.; Algethami, F.K.; Shah, R.K.; Saad, F.A.; Munshi, A.M.; Rehman, K.u.; Khezami, L.; Abdelrahman, E.A. Calcium Ferrite Nanoparticles: A Simple Synthesis Approach for the Effective Disposal of Congo Red Dye from Aqueous Environments. *Inorganics* **2024**, *12*, 69. [CrossRef]
6. Wang, N.; Wu, Y. First-Principles Investigation into the Interaction of H_2O with α-$CsPbI_3$ and the Intrinsic Defects within It. *Materials* **2024**, *17*, 1091. [CrossRef]
7. Hantoko, R.; Anggono, A.D.; Lubis, A.M.H.S.; Ngafwan. Microstructural Analysis of Friction Stir Welding Using CuZn and Zn Fillers on Aluminum 6061-T6: A Comparative Study. *Eng. Proc.* **2024**, *63*, 6. [CrossRef]
8. Chen, Y.; Li, A.; Jiang, S. Wettability and Mechanical Properties of Red Mud–Al_2O_3 Composites. *Materials* **2024**, *17*, 1095. [CrossRef]