



Memorias

First Iron Oxide Workshop

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VI Colombian Mössbauer Spectrometry School

Linking Geology, Medicine, Energy and Biotechnology



Sello Editorial
**UNIVERSIDAD
DEL ATLÁNTICO**

Memorias

First Iron Oxide



**VI Colombian Mössbauer
Spectrometry School: Linking Geology,
Medicine, Energy and Biotechnology**

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Vicerrectoría de Investigaciones, Extensión y Proyección Social
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Linking Geology, Medicine,
Energy and Biotechnology

Memorias del Evento

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Memorias del Evento

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Reynel Cárdenas, Valeria Quintana, Kimberlly Orozco, Jean Ospino y Melissa Quevedo, a los estudiantes de Física: Javier Molina y Ángel Pérez, y al estudiante de Química Carlos García.

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First Iron Oxide



Workshop

**VI Colombian Mössbauer
Spectrometry School :**
Linking Geology, Medicine, Energy
and Biotechnology

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Presentation

The First Iron Oxide Workshop investigates the diverse range of iron oxide particles produced from water reactions under varying redox and pH conditions. These particles include magnetite, maghemite, goethite, hematite, and akaganeite, and have applications in academia, water treatment, electronics, new energy production, cosmetics, medicine, and the paint industry. Iron oxide particles are highly adaptable due to their minute scale, typically under 100 nm, and high reactivity due to their large surface area. In biomedicine, these particles have shown extraordinary potential in various applications, including magnetic hyperthermia, contrast agents for MRI imaging, precise drug delivery systems, and gene therapy. Moreover, iron oxides possess intrinsic attributes that make them highly desirable for water treatment applications, such as cost-effectiveness, redox adaptability, magnetic properties, and efficient adsorption. Additionally, the formation of iron ore and the subsequent oxidation of minerals, such as magnetite, show potential as sources for generating hydrogen gas (H₂). Extensive research in recent decades has focused on synthesising iron oxide particles and understanding their natural origins, size, shape, reproducibility, and properties. Advanced techniques, such as Mössbauer spectroscopy and synchrotron methods, have been employed. The workshop covers a diverse range of topics.

The Sixth Colombian School of Mössbauer Spectroscopy serves as a platform for knowledge sharing and collaboration among Research Groups and international experts. The event offers fundamental and advanced courses in Mössbauer Spectroscopy, as well as highlighting advancements in instrumentation. Mössbauer Spectroscopy is an academic technique that has been playing a key role in unravelling the atomic, nuclear, chemical and magnetic intricacies of matter since the discovery of the Mössbauer effect in the 1950s. Its far-reaching applications span solid-state physics, magnetism, metallurgy, chemistry,

and biophysics. The primary goal of the School remains: to maintain the prominence of Mössbauer spectroscopy, particularly among students of science and engineering disciplines, by capitalising on its low-cost appeal and its diverse contributions to many fields.

The First Iron Oxide Workshop explores the versatile realm of iron oxide particles arising from water reactions under diverse redox and pH conditions. These particles, encompassing magnetite, maghemite, goethite, hematite, and akaganeite, find relevance across academia, water treatment, electronics, new energy production, cosmetics, medicine, and the paint industry. Their minute scale, typically under 100 nm, coupled with heightened reactivity due to expansive surface area, underpins their adaptability. Within biomedicine, these iron oxide particles showcase extraordinary potential in applications like magnetic hyperthermia, contrast agents for MRI imaging, precise drug delivery systems, and gene therapy. Furthermore, the intrinsic attributes of iron oxides, such as cost-effectiveness, redox adaptability, magnetic properties, and efficient adsorption, make them highly desirable for water treatment applications. Iron ore formation and the subsequent oxidation of minerals like magnetite appear to hold promise as sources for generating hydrogen gas (H₂). Extensive research in recent decades has focused on synthesising iron oxide particles and understanding their natural origins, size, shape, reproducibility, and properties. Advanced techniques, such as Mössbauer spectroscopy and synchrotron methods, have been employed. The workshop covers a diverse range of topics, such as:

- Mössbauer spectrometry school
- Mössbauer spectrometry applications
- Iron characterization
- Industrial applications
- Water treatment
- Iron and medicine
- Energy and environment

Below, you will find a collection of extended abstracts of the subjects presented by the speakers.

A note of clarification. Participants were requested to submit their abstracts adhering to specific guidelines on format, typography, style, and other academic conventions. We have meticulously followed these guidelines to ensure uniformity and consistency in formatting. However, it is important to emphasise that authorship and responsibility for the content and presentation of the resulting articles rest solely with their respective authors, despite possible variations in adherence to the prescribed parameters.

Mössbauer Spectrometry School

Introducción Espectroscopía Mössbauer: El efecto Mössbauer y Espectrometría Mössbauer con ^{57}Fe

Prof. Sebastián Trujillo
(*Universidad del Valle, Colombia*)

Interacciones hiperfinas

Prof. Cesar Barrero
(*Universidad de Antioquia, Colombia*)

De la estructura hiperfina al ajuste del espectro Mössbauer

Dr Jean Marc Greneche
(*IMMM, CNRS DR em., Francia*)

Instrumental aspects of Mössbauer spectroscopy

Prof. Alvaro Velásquez
(*Universidad EAFIT, Colombia*)

Espectrometría Mössbauer bajo campo magnético y preparación de muestra

Dr Jean Marc Greneche
(*IMMM, CNRS DR em., Francia*)

Mössbauer spectroscopy: experimental techniques

Prof. Jesús Tabares
(*Universidad del Valle, Colombia*)

Introducción Espectroscopía Mössbauer: El efecto Mössbauer y Espectrometría Mössbauer con ^{57}Fe

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La espectroscopia Mössbauer es una técnica avanzada en el campo de la física y la química que permite estudiar las propiedades de los núcleos atómicos en un nivel microscópico. Nombrada en honor al físico alemán Rudolf Mössbauer, esta técnica se basa en el fenómeno del efecto Mössbauer, que ocurre cuando un núcleo atómico emite o absorbe radiación gamma sin perder energía por retroceso. Esto permite un análisis preciso de la estructura electrónica y magnética de los materiales, así como de los estados de oxidación y el entorno químico de los átomos en una muestra.

La espectroscopia Mössbauer se utiliza ampliamente en diversas áreas de investigación, incluyendo la física de materiales, la geología, la metalurgia, la biología y la química. Proporciona información valiosa sobre la estructura y la dinámica de los materiales a nivel atómico, lo que ayuda a comprender mejor las propiedades y el comportamiento de sustancias específicas.

Topic: Mössbauer spectrometry school.

Interacciones hiperfinas

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El análisis de la estructura hiperfina del espectro Mössbauer hace parte de las bases teóricas para las aplicaciones del efecto Mössbauer. La estructura hiperfina es una pequeña perturbación en los niveles de energía del núcleo debido a su interacción con campos eléctricos (homogéneos e inhomogéneos) y magnéticos de origen extranuclear. En esta charla, explicaremos las interacciones isomérica, cuadrupolar y magnética y como estas se pueden correlacionar con las propiedades fisicoquímicas del material bajo estudio.

Keywords: Espectroscopía Mössbauer, interacciones hiperfinas

Topic: Mössbauer spectrometry school

De la estructura hiperfina al ajuste del espectro Mössbauer

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La idea de esta presentación es comprender cómo ajustar un espectro Mössbauer con (i) la atención dedicada a la optimización de las condiciones de registro y las estadísticas, (ii) con el tratamiento matemático de la estructura hiperfina, (iii) la correlación entre estos resultados matemáticos con las propiedades estructurales de la muestra, (iv) la estimación de las barras de incertidumbres de todos los parámetros hiperfinos y con (v) una presentación de los programas de ajuste más utilizados.

También discute (i) los efectos del espesor de la muestra en términos de efectos de polarización, (ii) la presencia de orientación preferencial (cuadrupolar y magnética) y (iii) los espectros con líneas ensanchadas.

Keywords: Mössbauer spectroscopy

Topic: Mössbauer spectrometry school

Instrumental aspects of Mössbauer spectroscopy

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This presentation covers the basic concepts concerned with the instrumentation of a Mössbauer spectrometer for room temperature operation, both in transmission mode as internal conversion electron mode. A brief description of the operation of the main modules of the spectrometer is presented and some low-cost modules of the spectrometer developed locally are presented [1,2]. The presentation also seeks to motivate the use of Mössbauer spectroscopy as a very useful technique to support the research of magnetic and structural properties of samples containing Mössbauer isotopes [3].

Keywords: Mössbauer spectrometer, CEMS camera, low-cost instrumentation, Mössbauer spectroscopy

Topic: Mössbauer spectrometry school

References

- [1] Velásquez A. A., Arroyave M. Implementation of a preamplifier and amplifier system for radiation detectors used in Mössbauer spectroscopy. *Hyperfine Interactions* 2014; 224: 65-72.
- [2] Velásquez A. A., Carmona A., Velásquez D., Angel L. Design and construction of an electromechanical velocity modulator for Mössbauer spectroscopy. *Hyperfine Interactions* 2011; 202: pages 63-71.
- [3] Implementation of a platform for the remote Access to a transmission Mössbauer spectrometer. *Hyperfine Interactions* 2019; 240(12): pages 1-9.

Espectrometría Mössbauer bajo campo magnético y preparación de muestra

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La primera parte se dedicará a la preparación de las muestras para optimizar las condiciones de registro en función de la morfología de los materiales (polvos, películas finas, ferrofluidos, etc.).

Además de la espectrometría Mössbauer convencional en geometría de transmisión, una presentación de la espectrometría Mössbauer bajo campo magnético recordará en primer lugar las condiciones instrumentales y experimentales para optimizar la adquisición de espectros en estas condiciones, y a continuación la motivación de la utilización de esta técnica para estudiar ciertas propiedades de materiales magnéticos cristalinos y/o amorfos, o incluso nanomateriales para estudiar los fenómenos de relajación superparamagnética.

Keywords: Mössbauer spectroscopy

Topic: Mössbauer spectrometry school

Mössbauer spectroscopy: experimental techniques

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Mössbauer spectroscopy (MS), is a nuclear technique based on the discovery of the emission and absorption of gamma photons without energy loss due to nuclear recoil, made by R.L. Mössbauer in 1958, which allows the quantification of hyperfine nuclear interactions and is applicable to the study of very diverse problems, both in Nuclear Physics, State Physics, Solid, Chemistry, Geology, Biology, etc.

In Mössbauer spectroscopy, most experiments are carried out in transmission geometry by incident the beam of γ rays emitted by the source and modulated by the Doppler effect on the sample or absorber so that the counter detects only the radiation that has passed through the sample. At certain Doppler velocities of the source, the energy of the γ radiation will coincide with that of the corresponding nuclear level of the sample and resonant absorption will take place, causing a decrease in the number of detected counts. In this work a description of each of the components of the spectrometer is made. Emphasis is placed on the characteristics that sources must have. The de-excitation process of a nucleus that has absorbed a gamma photon is discussed, explaining the internal conversion mechanisms and its usefulness in the study of surfaces using conversion electron Mössbauer spectroscopy (CEMS). A brief consideration is made about the characteristics of the

samples, specifically for Mössbauer spectroscopy of ^{57}Fe . Components of nuclear instrumentation used is presented, including the detectors characteristics, the preamplifiers and amplifiers for conforming the pulses produced in the detector. At this point the pulse height analyzer (PHA) function and the selection of counts or nuclear events recorded by the detector and counted by the multichannel are presented. A discussion is included about the speed modulation device or driver, its operation in constant acceleration mode and the synchronism of this movement with the multichannel function of the data collection system in order to represent the absorption spectrum (or emission if we use conversion electrons). Some examples of spectra are presented, the main one being that of alpha iron, which is used for calibration of the spectrometer.

Keywords: Mössbauer Spectroscopy, Hyperfine interactions, nuclear instrumentation

Topic: Mössbauer spectrometry school

References

- [1] Gütlich Philipp, Bill Eckhard and Trautwein Alfred X. Mössbauer Spectroscopy and Transition Metal Chemistry, Fundamentals and Applications, Springer, 2011.
- [2] May Leopold, An introduction to Mössbauer Spectroscopy, Plenum Press, NY, 1971.

Mössbauer Spectrometry Applications

Conferences

Use of Mössbauer spectrometry to study permanent magnets and magnetocaloric materials

Prof. Sebastián Trujillo
(*Universidad del Valle, Colombia*)

Mössbauer spectroscopy applied to the study of 1:12 permanent magnets and exchange coupling in MnAl/FeC

Prof. Ligia Edith Zamora Alfonso
(*Universidad del Valle, Colombia*)

Iron oxides and oxyhydroxides explored with Mössbauer spectroscopy: some achievements and future perspectives

Prof. Cesar Barrero
(*Universidad de Antioquia, Colombia*)

Aleaciones FeMnAlC obtenidas para aplicaciones del corte de caña de azúcar

Prof. Germán Pérez
(*Universidad del Valle, Colombia*)

Design, construction and commissioning of a “melt spinning” system for the production of metal alloys

Prof. Jesús Tabares
(*Universidad del Valle, Colombia*)

Use of Mössbauer spectrometry to study permanent magnets and magnetocaloric materials

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Permanent magnets (PMs) and magnetocaloric materials (MMs) are essential components in modern technological applications for power generation and magnetic refrigeration. As these technologies become more sophisticated, the demand for PMs and MMs increases. The most relevant magnets and magnetocaloric materials on the market are those based on Nd-Fe-B and La-Fe-Si alloy. However, the impact of the economic crisis on rare earth prices in 2011, led to the search for new PMs and MMs formed by low rare earth concentration or rare earth free nanocomposites, where their magnetic properties are usually optimized through nanostructured processes (coercivity mechanisms). In this talk, the most important phenomenology to consider in the study around

the production of new nanostructured rare-earth and rare-earth-free PMs and MMs will be presented in order to advance in the solution of this limitation. For this purpose, we will show the main production routes and research results of the magnetic and structural behavior of these different alloys that allow us to understand and control the complex interactions that arise in PMs and MMs, which require a high-quality material synthesis.

Keywords: Permanent Magnets, Magnetocaloric Materials, Melt Spinning.

Topic: Mössbauer spectrometry school

References

- [1] J. Cui, M. Kramer, L. Zhou, F. Liu, A. Gabay, G. Hadjipanayis, B. Balasubramanian, D. Sellmyer, Current progress and future challenges in rare-earth-free permanent magnets, *Acta Mater* 158 (2018) 118–137. <https://doi.org/10.1016/j.actamat.2018.07.049>.
- [2] H. Martínez-Sánchez, J.D. Gámez, J.L. Valenzuela, H.D. Colorado, L. Marín, L.A. Rodríguez, E. Snoeck, C. Gatel, L.E. Zamora, G.A. Pérez Alcázar, J.A. Tabares, Optimized Route for the Fabrication of MnAlC Permanent Magnets by Arc Melting, *Molecules* 27 (2022) 8347. <https://doi.org/10.3390/molecules27238347>.
- [3] K.P. Su, S.L. Hu, H.O. Wang, S. Huang, X.X. Chen, J.J. Liu, D.X. Huo, L. Ma, Z.W. Liu, Structural and magnetic properties of Mn₅₀Al₄₆Cu₄C₃ flakes obtained by surfactant-assisted ball milling, *Mater Res Express* 6 (2019) 106125. <https://doi.org/10.1088/2053-1591/ab4227>.

Mössbauer spectroscopy applied to the study of 1:12 permanent magnets and exchange coupling in MnAl/FeCo

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The study of permanent magnets (PMs) is very important because of their wide variety of technological applications in many industries, such as consumer electronics, transportation, military, electric (hybrid) vehicles, wind turbines, air conditioners, and hard-disk drives. The increasing importance of permanent magnets in modern society has resulted in renewed interest in the design and discovery of new permanent magnet materials that are cheaper, use less rare earth elements, and can be used in clean energy applications. In this presentation, the results of the research conducted on two systems that are considered PM are shown.

This work is focused on the use of the Mössbauer spectroscopy in two different systems of permanent magnets. The first system is the ReTm_{12} type, where Re is a rare earth element and Tm is a transition metal. The effects of Nd substitution by Ce and follow by a nitrogenating were studied. The structural, hyperfine, and magnetic properties of $(\text{Nd}_{1-x}\text{Ce}_x)_{1.1}\text{Fe}_{10}\text{CoTi}$ with $x = 0, 0.5, \text{ and } 1$ system were analyzed. X-ray diffraction analysis allowed the identification of tetragonal ThMn_{12} -

type structure, rhombohedral $\text{Th}_2\text{Zn}_{17}$ -type structure, and the Cu_2Mg -type cubic structure. The Mössbauer spectra were fitted using seven sextets and a small quadrupolar component. The sextets were associated with the Fe sites in the ThMn_{12} -type and $\text{Th}_2\text{Zn}_{17}$ -type phases and the quadrupolar component of the Cu_2Mg structure. The mean field, $\langle B_{\text{hf}} \rangle$, improved for all the alloys after the nitrogenating process. The effect of the nitrogenating process on intrinsic magnetic properties such as saturation magnetization, anisotropy field, the magnetocrystalline anisotropy constant, and Curie temperature of $(\text{Nd}_{1-x}\text{Ce}_x)_{1.1}\text{Fe}_{10}\text{CoTi}$ ($x = 0.0, 0.5 \text{ and } 1$) alloy systems was also analyzed. The best magnetic properties were found for the $\text{Nd}_{1.1}\text{Fe}_{10}\text{CoTiNy}$ compound, for which it was estimated a saturation magnetization of $153.3 \text{ Am}^2\text{kg}^{-1}$, anisotropy field of 10.3 T , anisotropy constant of 5.98 MJm^{-3} , and Curie temperature of 768.9 K .

The second studied system is one in which exchange coupling between hard and soft magnetic phases is present, which is known as an exchange spring magnet. They appeared to be an alternative for the development of high energy product permanent magnets. In this study, the exchange coupling of MnAlC/FeCo was characterized. The hard phase (MnAlC) has high coercivity, and the soft phase (FeCo) has high saturation magnetization. The hard and soft phases interact through their interface via exchange coupling, and the samples were obtained using a solid-state procedure. The magnetic materials were sintered using different ratios of hard and soft magnetic phases and different sintering temperatures and times to improve their magnetic properties. The magnetic exchange coupling between MnAlC and FeCo was confirmed by the hysteresis loop. The best result was obtained for MnAlC/FeCo (95/5 wt%) sintered at $500 \text{ }^\circ\text{C}$ for 30 min, for which the magnetic properties were $\mu_0 H_c = 0.277 \text{ T}$, $M_s = 76.43 \text{ Am}^2/\text{kg}$ and $(BH)_{\text{max}} = 5.57 \text{ kJ/m}$.

Keywords: Permanent magnets, Mössbauer spectroscopy, exchange spring magnet

Topic: Mössbauer spectrometry applications

References

- [1] Hugo Martínez Sánchez, Daniel Salazar, Ligia Edith Zamora, Juan Sebastián Trujillo Hernández, Jesús Anselmo Tabares, German Antonio Pérez Alcázar. Mössbauer spectroscopy in the system $(\text{Nd}_{1-x}\text{Ce}_x)_{1.1}\text{Fe}_{10}\text{CoTi}$ with ThMn_{12} structure. *Hyperfine Interactions*, 2020, VOL. 241, p. 1-11.
- [2] H. Martínez Sánchez, L. E. Zamora Alfonso, J. S. Trujillo Hernández, D. Salazar Jaramillo, and G. A. Pérez Alcázar. Effect of Nitrogenation on the Intrinsic Magnetic Properties of the Compounds $(\text{Nd}_{1-x}\text{Ce}_x)_{1.1}\text{Fe}_{10}\text{CoTi}$ IEEE transactions on magnetics, 2020, VOL. 56, p. 1-5.
- [3]. H. Martinez Sanchez, L.E. Zamora Alfonso, J.S. Trujillo Hernandez, G.A. Perez Alcazar. Evidence of exchange coupling in -MnAlC/FeCo system *Journal of Magnetism and Magnetic Materials*, 2019, 473 221–227.

Iron oxides and oxyhydroxides explored with Mössbauer spectroscopy: some achievements and future perspectives

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Iron oxides and oxyhydroxides are very abundant in nature and have multiple uses and applications. These compounds have long been studied by Mössbauer spectroscopy. This technique is routinely used by several laboratories, and it has been proved to be very valuable not only for identification, but for retrieving important information regarding physico-chemical characteristics of the iron compounds. In this presentation, we will show some Mössbauer results of our group particularly on the synthetic versions of goethite, magnetite and akagenite. Furthermore, some works related with the applications of these compounds for the removal of some water contaminants and the corrosion process of iron and steels will be presented. Future perspectives in Mössbauer research regarding iron oxides will be outlined.

Keywords: iron oxides, iron oxyhydroxides, Mössbauer spectroscopy

Topic: Mössbauer spectrometry applications

Aleaciones FeMnAlC obtenidas para aplicaciones del corte de caña de azúcar

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In this work we reported the preparation process and the characterization of their mechanical, magnetic, and structural properties of some alloys of the Fermanal (FeMnAlC) type. The prepared alloy series Fe-18Mn-xAl-0.7C and Fe-28Mn-xAl-0.7C in wt. %, with $x = 0, 3, 6,$ and 9 , were obtained by melting in an induction furnace, in adequate quantities to obtain the desired compositions, scraps of the alloys AISI 1020 and 1045, high- and low-carbon ferro-manganese, ferro-silicon, ferro-molybdenum, and copper and aluminium as pure elements. After the melting process, the liquid metal was poured into a sand mold covered with zirconium paint to obtain 150X100X35 mm size thick plates of as-cast samples which were then hot-forging at 1100 °C in different steps up to obtain 50% of the original thickness. From the laminas it was cut samples for be characterized by X-ray fluorescence (XRF) and optical emission spectroscopy (OES) techniques,

XRD, Mössbauer spectrometry (MS), SEM, and electron backscatter diffraction (EBSD) characterizations, and for microhardness, and low-stress abrasive wear experiments. The X-ray fluorescence (XRF) and optical emission spectroscopy (OES) techniques proved that the chemical compositions of the produced samples are close enough to the targeted chemical compositions. By SEM it was observed, in all the samples, the typical austenite microstructure and in some cases (for samples with big Al content) it was detected also the ferritic microstructure. By EBSD it was determined that dynamic recrystallization occurs due to strain-induced boundary migration and is strongly influenced by the aluminium content of the alloy and its stacking failure energy (SFE), increasing the aluminium content will generate greater nucleation sites, favouring the refinement of grains in the material and achieving a crystalline structure of random crystallographic orientation. MS spectra of the alloys with $x \leq 6$ were fitted with 3 singlets with different isomer shifts and spectral areas attributed to three different austenite phases, and those with $x = 9$ with these three singlets and a magnetic hyperfine field distribution (MHFD) associated to the disordered ferrite phase. XRD patterns of the $x \leq 6$ samples were refined with the peak sequence of three fcc structures with small differences in their lattice parameters, and that with $x = 9$ with an additional bcc structure. This is a duplex sample due its patter was refined with the fcc and bcc structures. These results are in accord with those of the MS measurements. The three fcc structures correspond to the three singlets and the bcc structure to the MHFD. The presence of the three fcc phases is explained by a partial spinodal decomposition that normally appears in many fcc structures when they are cooled from high temperatures. The original fcc structure with intermediate lattice parameter corresponds to the as-cast sample, which partially decompose in other two fcc structures, one with small lattice parameter corresponding to one with small quantity of solute atoms (Al and C) and the other with high lattice parameter due the bigger quantity of solute atoms (Al and C). Finally, the results of the microhardness experiments and those of the low-stress abrasive wear experiments, permitted to show that four of the prepared samples present better mechanical properties than those of the AISI D2 and AISI 9260 steels, which are those used by the fabricants of the sugar cane cutting blades in Colombia.

Topic: Mössbauer spectrometry applications

Design, construction and commissioning of a “melt spinning” system for the production of metal alloys

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It is well known materials are the foundation of experimental magnetism and practical applications depend on the nature and form of a material. The great majority of laboratory studied specimens are man-made, often resulting of complex fabrication processes. One of the most common and efficient techniques used at the level of basic research and industrial production is the melt spinning process. With this process ribbons can be manufactured continuously from the molten material with amorphous or nanocrystalline microstructure.

This work presents the design, construction and commissioning of a “melt spinning” system for the production of metal alloys for use in permanent magnets. We specifically describe the manufacturing of the vacuum chamber and the steps to communicate the movement to the copper wheel while preserving the vacuum using a magnetic coupler manufactured especially for our device. On the other hand, in the melt spinning, the metal alloy is first melted inside a crucible (quartz tube) using an induction furnace and then the molten material is expelled through a small hole at the lower end of the crucible or

nozzle (~ 0.6 mm diameter), by applying an overpressure (~ 0.2 bar) of gas (Ar). The expelled molten material is projected on the surface of a rotating copper wheel, located at a small distance from the nozzle (~1 mm). Likewise, the manufacture of the crucible positioning system and the automatic injection of the overpressure gas are presented. The entire process is carried out in an inert Ar atmosphere (pressure ~0.8 bar). In the small space between the outlet nozzle of the molten material and the surface of the rotating wheel, a deformed drop is formed due to the surface tension of the material. When the material in the drop comes in contact with the rotating wheel, it solidifies quickly and produces a continuous ribbon fed by material from the nozzle. From the control of the flow of the molten metal through the nozzle and the solidification speed (rotation speed of the copper wheel) are fundamental parameters in the expected properties of the material produced [1-3].

It is including current work in permanent magnets in our research group using this apparatus.

Keywords: Rapid solidification, melt spinning, metallic alloys.

Topic: Mössbauer spectrometry applications

References

- [1] E. A. Theisen, M. J. Davis, S. J. Weinstein, and P. H. Steen, “Transient behavior of the planar-flow melt spinning process,” *Chem. Eng. Sci.*, vol. 65, no. 10, pp. 3249–3259, 2010.
- [2] S. Sohrabi, H. Arabi, a. Beitollahi, and R. Gholamipour, “Planar Flow Casting of Fe₇₁Si_{13.5}B₉Nb₃Cu₁Al_{1.5}Ge₁ Ribbons,” *J. Mater. Eng. Perform.*, Feb. 2013.
- [3] M. Srinivas, B. Majumdar, D. Akhtar, a. P. Srivastava, and D. Srivastava, “Influence of wheel speed during planar flow melt spinning on the microstructure and soft magnetic properties of Fe_{68.5}Si_{18.5}B₉Nb₃Cu₁ ribbons,” *J. Mater. Sci.*, vol. 46, no. 3, pp. 616–622, Oct. 2010.

Iron Oxide Workshop: Iron Characterization

Conferences

Magnetic dipolar interactions in Fe-based nanoparticles ensembles: fundamentals, effects, analysis of experimental results and potential applications

Prof. Francisco H. Sánchez

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Structural and Physical properties of Fe nanostructures

Prof. Jean Marc Greneche

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Integrating nontraditional isotope measurements and synchrotron-based absorption techniques into your research

Prof. Anthony Chappaz

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Chemical surface properties and nano effect of Fe oxides

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Machine Learning Insights into Band Gap Dynamics and Oxygen Vacancy Formation

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Ab-initio study of anomalous hall effect in the altermagnet Fe₂O₃

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Magnetic dipolar interactions in fe-based nanoparticles ensembles: fundamentals, effects, analysis of experimental results and potential applications

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Condensates with continuous magnetism present an internal demagnetizing field which depends on their shape as well as on their magnetization degree and direction. As a consequence, their magnetic response is a function of the effective field, i.e. the sum of applied plus demagnetizing fields. The theory of demagnetizing fields is well known for these continuous bodies, where magnetic poles are located just at the surfaces [1]. Dispersions of magnetic nanoparticles in powders, colloids, gels, solids, etc., i.e. magnetic heterogeneous materials, may also experience strong dipolar interactions which lead to demagnetizing and even magnetizing fields [2]. In this tutorial, experimental results and models to predict the effects of these interactions in heterogeneous samples

are presented and discussed. As a consequence of these effects it turns out that it is necessary to give details of sample shape and orientation when reporting magnetic results from nanoparticle systems. Conversely, from the experimental results it is possible to obtain information on the superstructures that nanoparticles may form and on their dependence on the applied field. In this way dipolar interactions between nanoparticles become nanosensors on the materials state and evolution.

Keywords: magnetic dipolar interactions, nanoparticle dispersions, effective demagnetizing tensor

Topic: Iron characterization

References

- [1] B. D. Cullity and C. D. Graham, Introduction to magnetic materials, Wiley 2009.
[2] F. H. Sánchez et al., Dipolar interaction and demagnetizing effects in magnetic nanoparticle dispersions: Introducing the mean-field interacting superparamagnet model, Physical Review B 95, 134421 (2017), DOI: 10.1103/PhysRevB.95.13442

Structural and Physical properties of Fe nanostructures

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After discussing the main characteristics of artificial and natural nanostructures, including nanoparticles, multilayers, and nanostructured materials, we review the questions that need to be resolved in order a better understanding their structural and physical properties. The first step is to establish correlations between their physical properties and their size, the morphology and chemical composition of the crystalline grains, the thickness of the grain boundaries and the quality of the interfaces, respectively. The second step is to distinguish the nature of surfaces and grain boundaries and to understand their role on the magnetic properties.

To illustrate this strategy, we give some examples based on results obtained by ⁵⁷Fe Mössbauer spectrometry, a local probe technique well appropriate to the study of these complex Fe-containing nanomaterials. We show that this fundamental approach was necessary to better understand the relationship between the morphology of nanostructures and their physical and chemical properties and also to characterize some natural and highly complex nanostructures resulting from corrosion science, geology, environmental science, archeology, agriculture.

Topic: Iron characterization

Integrating nontraditional isotope measurements and synchrotron-based absorption techniques into your research

most of the geoscientists keep relying mainly on bulk elemental concentration and sometimes isotope ratios but often neglect two other aspects: speciation and spatial distribution. Unfortunately, these omissions can lead to major misunderstanding of the processes at play. Using synchrotron-based absorption techniques to characterize the speciation of trace elements and Fe oxides bring new insights that strongly enhance our understanding of the processes at play.

Trace Element Molecular Geochemistry consists in combining measurements of the trace element concentration, spatial distribution, isotope ratios and speciation within specific discrete phases. Two parts compose my keynote. Part 1 will introduce the basic concepts necessary to understand non-traditional isotopes and synchrotron-based absorption techniques. The second part will present case studies showing how applying a molecular geochemical approach can greatly enhance our comprehension of trace element – iron oxide systems.

Topic: Iron characterization

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Trace elements are ubiquitous. They can be found in all natural and engineered systems. Some are bio-essential micronutrients that support life, while others can be toxic to living organisms. To study the Earth's history and the origin of Life, many are used as paleo proxies to reconstruct ancient environmental conditions. To support the Green Energy Transition, critical elements are essential for our modern societies aiming to promote a Sustainable Earth. Iron (Fe) oxides and oxyhydroxides are widespread at the Earth's surface and play a major role in many biogeochemical processes. Examining the interactions between trace elements and Fe (oxyhydr)oxides is highly valuable for Earth and environmental sciences, material sciences, (micro)biology, physics, and medical sciences. When studying trace element – Fe oxide interactions,

Chemical surface properties and nano effect of Fe oxides

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After discussing the main structures of natural iron oxides, including nanoparticles, we will review their surface chemistry, namely their proton surface charge, their surface complexation, without or with electron transfer. Each of these topics will be discussed at the light of (i) wet chemistry, (ii) structure of surface complex and reactive surface sites and (iii) applications in the field of environmental sciences (heavy metal or oxyanion contaminations, river natural attenuation or on the opposite mine contamination by particles). Rates and mechanisms of important reactions in the cycling of electrons at the earth Surface via the geochemical transformations of iron have been identified using XAFS and Mössbauer spectrometry. The ability of Fe-bearing solids surfaces to interact chemically, through surface complexation, and ligand exchange mechanisms, with reductants such as FeII, and oxidants such as Se, U, Tc, Co, Eu, and O₂ facilitates electron transfer as well as particule dissolution and precipitation. Various pathways have been assessed on the basis of laboratory experiments for application to natural and engineered systems. FeII in the structure of oxides (e.g., inorganic or bio-magnetite Fe₃O₄) as well as FeII surface complexes, such as on clay mineral edges, are very efficient reductants from a thermodynamic as well as from a kinetic point of view. We will discuss some examples of societal importance based on combined results

obtained by wet chemistry, XAFS spectroscopy, SEM-EELS microscopy and ⁵⁷Fe Mössbauer spectrometry cutting edge techniques, particularly well appropriate to study complex Fe-containing nanomaterials found in environmental science, archeology, agriculture. We will discuss the size effect on the Fe oxide physical and chemical properties, i.e., the “nano effect”. Indeed, the cycling of iron in various Earth surface reservoirs (aquifer, soils, sediments) depends on Fe-bearing solid high surface-area-to-volume ratio. We show that this fundamental approach to Fe oxide reactivity is necessary to better understand the relationship between particle nanostructures and their physical and chemical retention properties. Finally we will discuss some questions that need to be resolved in order to further better understand their reactivity in the environment.

Topic: Iron characterization

Machine Learning Insights into Band Gap Dynamics and Oxygen Vacancy Formation

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Aiming to predict compounds with oxygen vacancy formation, we employ machine learning models to determine the relationship between bandgap existence and oxygen vacancy formation in gapped systems, considering simple materials and atomic properties. Firstly, we explore the impact of semiconductor band gaps on potential applications. Utilizing the interpretable machine learning model, the multiVariate dAta eXplanation (VAX) method, researchers derive insights from a dataset exceeding 10,000 entries extracted from the Materials Project. Atomic properties, including electrons, electronic affinity, and orbital energies, inform random forest models revealing the influence of symmetry and atomic orbital energy on band gap directness. Sub-group analyses based on structures like zincblende, rocksalt, wurtzite, and perovskite highlight the pivotal role of symmetry. Next, we focus on oxygen vacancies in oxide materials, showcasing the development of high-throughput point-defect calculation codes. By analyzing 937 oxides, researchers harness machine-learning regression models to predict vacancy formation energies, underscoring the crucial role of oxygen vacancies in advancing oxide material discovery.

Topic: Iron characterization

Ab-initio study of anomalous hall effect in the altermagnet Fe_2O_3

understanding the anomalous Hall effect and the spin Hall effect using Berry-phase and spin Berry-phase concepts, respectively. These theoretical perspectives have led to predictions of a large intrinsic anomalous Hall effect and spin polarized currents in altermagnets with broken effective time-reversal symmetries (e.g. collinear antiferromagnets RuO_2 and Fe_2O_3) [1,2]. In this work, we will present ab-initio calculations combined with symmetry analysis to show the generation of the anomalous Hall current in the altermagnetic phase of $\alpha\text{-Fe}_2\text{O}_3$ [3].

Keywords: Anomalous Hall effect, Altermagnet, Hematite

Topic: Iron characterization

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Spintronics is an analogue to electronics where the spin of the electron rather than its charge is functionally controlled for energy efficient devices. The generation of spin/charge currents without ferromagnetic or exotic/scarce materials is one of the biggest challenges for spintronic devices, and the anomalous/spin Hall effect could be a key in order to solve this problem. Recent development in experimental and theoretical studies have offered a framework for

References

- [1] L. Šmejkal et al., Crystal time-reversal symmetry breaking and spontaneous Hall effect in collinear antiferromagnets. *Sci. Adv.* 6, eaaz8809 (2020).
- [2] R. González-Hernández et al. Efficient Electrical Spin Splitter Based on Nonrelativistic Collinear Antiferromagnetism. *Phys. Rev. Lett.* 126, 127701 (2021).
- [3] E. F. Galindez-Rualez et al., Anisotropic magnetotransport realized in doped hematite. arXiv preprint arXiv:2310.16907 (2024).

Iron Oxide Workshop: Industrial applications

Conferences

Micromagnetic modelling of Fe-based alloys with potential applications as permanent magnets

Prof. Luis Rodríguez

(Universidad del Valle, Colombia)

Fabrication and characterization of magnetite microspheres obtained from mill scale in the steel Industry

Prof. Lorena Marín

(Universidad del Valle, Colombia)

Construction of phase diagrams for magnetic alloys using the renormalization method and neural networks

Juan E. Bedoya

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Micromagnetic modelling of Fe-based alloys with potential applications as permanent magnets

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Exchange-spring magnets represent a promising nanostructured magnetic material poised to address a primary challenge with widely used high-performance magnets: the reduction of rare-earth elements within their composition [1]. In an exchange-spring magnets, a nanostructured hard magnetic phase is combined with a nanostructured magnetic phase. Through inter-phase exchange coupling, we can engineer a nanocomposite magnet with an energy product, (BH)_{max}, surpassing that of the hard phase alone [2]. While exchange-spring magnets can be designed in bulk (technological applications demand bulk magnets), it is the thin film configuration that demonstrate superior performance [3].

In this talk, I will share preliminary findings from our micromagnetic simulations of thin-film exchange-spring magnets based on Nd₂Fe₁₄B (NdFeB, hard phase) and Fe₆₅Co₃₅ (FeCo, soft phase) systems. Micromagnetic simulations were conducted using Mumax3 software, a GPU-accelerated program enabling efficient simulations of magnetic hysteresis loops. Our investigation focused on the exchange spring coupling effect in NdFeB/FeCo bilayered and NdFeB/FeCo/NdFeB trilayered systems, with varying thicknesses of the FeCo layer from 2 to 12 nm. Our results indicate that, across most multilayered configurations studied here, the energy product exceeds that of a single-crystal NdFeCo layer. Additionally, a detailed analysis of magnetization switching mechanism reveals a partial decoupling of the soft film with increased FeCo thicknesses.

Keywords: Micromagnetic simulation, exchange-spring magnets, energy product

Topic: Magnetic modelling

References

- [1] Filip Ronning and Sam Bader. Rare earth replacement magnets. *J. Phys.: Condens. Matter* 2014; 26: 060301
- [2] J. P. Liu. Exchange-Coupled Nanocomposite Permanent Magnets. In book *Nanoscale Magnetic Materials and Applications* 2009; pages 309-335.
- [3] Hugo Martínez et. al. Scientific and Technological Analysis of Exchange-Spring Magnets: Applications and Trends. *Heliyon* 2024; submitted article.

Fabrication and characterization of magnetite microspheres obtained from mill scale in the steel Industry

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Despite being a very interesting industrial byproduct due to its high iron concentration (~72% by weight), its reuse in new production processes is low, with most of the scale ending up in landfills, posing a serious environmental risk due to the leaching of heavy metals into the soil. Thus, this work presents an alternative valorization of this byproduct: the obtaining of magnetite particles (Fe₃O₄), which are attractive in different industrial environments, offering a fast and economical route.

In this research, samples of mill scale provided by two Colombian steels were used. The materials were pulverized in a low-energy ball mill, sieved, and then fluidized in a flame from propane/oxygen combustion. The obtained materials and precursor scales were characterized using infrared spectroscopy (FTIR), X-ray diffraction (XRD), Mössbauer spectroscopy (MS), and scanning electron microscopy (SEM). The XRD and MS analysis allowed for the identification of the main crystalline phases in the scales: wustite, hematite, and magnetite. Following flame fluidization, SEM, XRD, and MS showed that the starting acicular particles transformed into microspheres with the main crystalline phase being magnetite (>96% by weight). SQUID magnetic measurements determined that the saturation magnetization and coercive field are between 84 – 94 emu/g and 22 – 23 Oe, respectively. Finally, it can be concluded that magnetite microspheres (Fe₃O₄) with sizes between 40 – 70 μm were successfully synthesized from two types of residues from the steel industry.

Keywords: Mill scale, magnetite, Fe₃O₄, magnetite microspheres

Topic: Iron Characterization

Mill scale is a layer of oxides that forms on the surface of steel during the hot rolling process. On average, between 35 and 40 kg of scale are produced for every ton of rolled steel.

Construction of phase diagrams for magnetic alloys using the renormalization method and neural networks

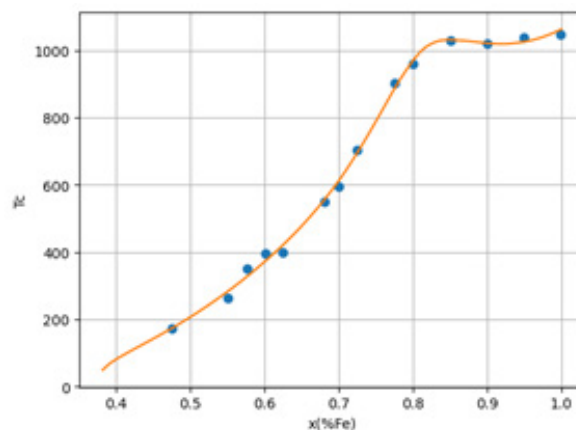


Figure 1: Theoretical phase diagram of the FeAl system using neural networks.

Additionally, by conducting a Monte Carlo simulation on the FeAl system, a second theoretical phase diagram was obtained using this method, but in contrast, employing a linear model without neural networks. A scale similar to that obtained in previous research is observed [1], providing a preliminary approximation to the theoretical model. In conclusion, the significance of this work lies not only in the discovery of a theoretical method to find magnetic phase diagrams but also in the potential to approximate the functional form of the Ising model's bonding energy.

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Using the Renormalization Group method in the Mean Field approximation (GRCM), starting from the Ising Hamiltonian and leveraging advancements in neural network adjustments, we aim to advance in constructing theoretical phase diagrams for the FeAl system. This is based on experimental data, yielding promising results at first glance, as depicted in Figure 1.

Keywords: Magnetism, Spin, Phase Diagram, Renormalization, Monte Carlo

Topic: Industrial applications

References

Juan Esteban Bedoya Rodríguez, Germán Antonio Pérez Alcázar. Diluted and random-bond Ising model and the Mean-field renormalization group (MFRG) method for the interpretation of the magnetic phase diagram of the Fe_xMn_{0.6-x}Al_{0.4} alloy series. Phys. Lett. A. 2023; volume: pages 1-4.

Iron Oxide Workshop: Iron and medicine

Conferences

Synthesis and characterization of magnetite-maghemite nanoparticles coated with chitosan, for biomedical applications

Prof. Alvaro Velásquez
(EAFIT, Colombia)

Design of nanoparticles for theranostics: synthesis strategy and positive impact of combining characterization techniques including Mössbauer spectrometry

Prof. Sylvie Begin
(Institut de Physique et Chimie des Matériaux de Strasbourg, France)

Characterization of magnetite superparamagnetic iron oxide nanoparticles containing Gd: dependence on the Fe(III)/Gd(III) ratio

PhD(c) Carolina Guida
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The key role of iron's redox chemistry in antibacterial clay minerals

Dr. Carolina Londono Michel
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Synthesis and characterization of magnetite-maghemite nanoparticles coated with chitosan, for biomedical applications

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Chitosan is a biocompatible and biodegradable polysaccharide, available in the shells of crustaceans [1] and highly promising for obtaining inorganic-organic type structures, also called composites, with applications in medicine, pharmacy and biotechnology [2,3]. In this work, we have obtained aqueous suspensions of spinel iron oxide nanoparticles stabilized with chitosan, with application in biomedicine. The nanoparticles were obtained by the coprecipitation method of Fe²⁺ and Fe³⁺ species in a

quaternized chitosan solution. Infrared spectroscopy and thermogravimetric measurements showed that the quaternized chitosan chains bind to the surface of the nanoparticles, the proposed binding mechanism being the link between the hydroxyl groups of the polysaccharide with the surface iron cations of the nanoparticles. Room temperature Mössbauer measurements showed that the nanoparticles are composed of two inverse spinel phases of magnetite and maghemite. Magnetization measurements showed a saturation magnetization of 8.5 A m² kg⁻¹, coercivity of 8 kA m⁻¹ and a saturation magnetic field of 200 kA m⁻¹, which is consistent with the presence of polymer chains bounded to the surface of the nanoparticles, reducing their specific saturation magnetization with respect to that of a crystalline and stoichiometric magnetite. Zeta potential measurements showed a narrow peak centered at 57 mV, indicating that nanoparticles are stable against aggregation in aqueous medium.

The potential cytotoxic effect of the nanoparticle suspension was determined using MTT and resazurin viability assays in cultures of the macrophage cell line J774. Our results indicate that J744 cells incubated for 24 hours tolerate up to 100 ppm of nanocomposite without significantly decreasing their viability. Therefore, our results support the hypothesis that the synthesized aqueous suspensions of magnetic nanocomposites are biocompatible, which opens a door to their use in future biomedical applications.

Keywords: Magnetite-maghemite nanoparticles, chitosan, Mössbauer spectroscopy

Topic: Iron Medicine

References

- [1] Lustraine C., Dwivany F.M, Suendo V., Reza M. Effect of chitosan and chitosan-nanoparticles on post harvest quality of banana fruits J Plant Biotechnol 2018; 45: pages 36–44.
- [2] Li G., Jiang Y., Huang K., Ding P., Chen J. Preparation and properties of magnetic Fe₃O₄-chitosan nanoparticles. J. Alloys Compd. 2008; 466: pages 451-456.
- [3] Silva A.C., Oliveira T.R., Mamani J.B., Malheiros S.M.F., Malavolta L., Pavon L.F., Sibov T., Amaro E., Tannús A., Vidoto E.L.G., Martins M.J., Santos R.S., Gamarra L.F. Application of hyperthermia induced by superparamagnetic iron oxide nanoparticles in glioma treatment. Int J Nanomedicine 2011; 6: pages 591-603.

Design of nanoparticles for theranostics: synthesis strategy and positive impact of combining characterization techniques including Mössbauer spectrometry

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Due to the wide range of applications for iron oxide nanoparticles (NPs), from nanoelectronics to nanomedicine, controlling their size, composition and shape on demand remains a major challenge, as these structural parameters are of utmost importance to deliver nanoparticles with magnetic

properties tailored to the targeted application. However, if the experimental parameters leading to different sizes and shapes are known, reproducibility of the synthesis is often difficult. There is currently a strong need to better understand the synthesis mechanism in order to better control the synthesis process and the design of nanoparticles. In nanomedicine, the aim is to synthesize NPs capable of combining diagnostic and therapeutic functions in a single formulation (theranostic NPs), enabling tumors to be imaged, treated and the effect of treatment to be monitored by imaging. NPs with a diameter of 20 nm are reported to be highly effective as contrast agents for MRI and as therapeutic agents by magnetic hyperthermia and photothermia, but their synthesis remains difficult as they often present a core-shell structure with a core of wüstite composition, detrimental to the desired theranostic properties.

In this context, we have studied the impact of the chemical nature of an iron precursor: iron stearate, on the synthesis of NPs and on the nucleation and growth mechanisms. Two iron stearate precursors with a lamellar structure were elaborated by coprecipitation and characterized. The study of their thermal decomposition, in particular by Mössbauer temperature spectrometry, showed that the seeds formed had a wüstite composition and that nucleation is the result of two reactions: i) the simultaneous catalyzed departure of two carboxylate chains and the reduction of Fe(III) to Fe(II) and ii) the condensation of these “activated” complexes leading to wüstite nuclei by a polymerization process.

We then studied the nucleation and growth mechanisms of NPs in more detail. The control of NP structure and size is often explained by LaMer theory, which implies a clear separation between the nucleation and growth stages. The events preceding the nucleation stage were investigated by combining different complementary in situ characterization techniques (liquid cell TEM, high-temperature TEM, SAXS/WAXS). This study revealed a new nucleation mechanism for the thermal decomposition method: instead of homogeneous nucleation in the solvent, nucleation occurs in vesicle-shaped “nanoreactors” that confine the reactants. This mechanism of nucleation in vesicles explains the wüstite composition of the seeds and the difficulty of obtaining nanoparticles larger than 15 nm with a homogeneous spinel composition. Mössbauer spectrometry has been a major characterization technique for confirming these different processes.

These studies, leading to a better understanding of nucleation and growth mechanisms, pave the way for improved control of the synthesis process for metal oxide nanoparticles and their properties.

Topic: Iron Medicine

Characterization of magnetite superparamagnetic iron oxide nanoparticles containing Gd: dependence on the Fe(III)/Gd(III) ratio

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Increasing levels of Gd have been detected in various natural water bodies in major cities around the world due to medical and industrial uses. Magnetic resonance imaging (MRI) contrast agents based on organic gadolinium(III) complexes appear to be the most widely used for signal enhancement of vessels and brain tumors. On the other hand, magnetite particles are a potent material for in situ remediation of contaminants and, in the medical field, are capable of MRI contrast enhancement and can be used as carriers for targeted drug or gene delivery, i.e. drug delivery systems. We report here first the synthesis route, structural characteristics, and some magnetic properties of Gd(III) containing magnetite nanoparticles solid solutions, evidenced by TEM, XRD, and ⁵⁷Fe Mössbauer spectrometry. The mean size and morphology of the nanoparticles seem to be independent of the Gd content, contrary to their mineralogical composition. The Mössbauer spectra at 300K and 77K show complex hyperfine structures resulting from a mixture of magnetite and maghemite coupled with superparamagnetic relaxation effects. Above 7% Gd, we observe a significant formation of antiferromagnetic goethite. Thus, Gd-doped nano magnetite MRI contrast agent should be limited to 1%-5% Gadolinium.

Keywords: Nanomagnetite, Gd doped magnetite, emerging contaminant, wastewater, MRI, Gadolinium, Magnetite
Topic: Iron and medicine

The key role of iron's redox chemistry in antibacterial clay minerals

clays and iron-sulfides, (e.g. nano-pyrite) sourced the reduced iron under acidic conditions. This leads to an overabundance of reduced iron, and ROS, in the medium, overpowering bacterial cells. In this talk, we will review the beginnings of natural antibacterial clay research and the cutting-edge advancements, attained by other researchers [e.g., 1], that have resulted in synthetic antibacterial minerals as promising therapies against dangerous bacterial infections on the skin.

Keywords: Antibacterial clays, Redox chemistry, Reactive Oxygen Species, Medical Geology

Topic: Iron and medicine

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The rise of antibiotic-resistant strains globally, and the pollution caused by excessive use of antibiotics, drive us to search for natural alternatives to pharmaceutical antibiotics. Antibacterial clays are minerals of $< 2 \mu\text{m}$ that inhibit bacterial growth in vitro. Iron's redox chemistry has played a crucial role in understanding the antibacterial mechanism and synthesizing high-purity minerals that mimic the natural effect. Methods from microbiology and geochemistry were combined to evaluate the mineral-microbe interactions that cause antibacterial effectiveness. The change in oxidation state of iron produces Reactive Oxygen Species (ROS) that negatively impact cellular structures and processes. Smectitic

References

[1] Morrison, K.D., Reiss, M.B., Tanner, T.D. et al. The application of synthetic antibacterial minerals to combat topical infections: exploring a mouse model of MRSA infection. *Sci Rep* 14, 1762 (2024). <https://doi.org/10.1038/s41598-024-52082-8>

Iron Oxide Workshop: Water Treatment

Conferences

Application of iron oxide nanoparticles for removal of pollutants

Prof. Adriana Herrera

(Universidad de Cartagena, Colombia)

Magnetic remediators as remarkable alternatives for real water treatments: current challenges and perspectives

Prof. Juan Adrian Ramos Guivar

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Retention potential of contaminants by (nano) magnetite in batch and microfluidic systems

Dr Evgenia-Maria Papaslioti

(Universidad de Huelva, España)

Utilization of akageneite nanoparticles for adsorption of heavy metals in water

Danis Gómez

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Magnetic iron-based nanoadsorbents for boron and phosphorus remediation

Prof. Edson Passamani Caetano

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Synthesis and characterization of nanocrystalline ferrites from the $Mn_{1-x}Zn_xFe_2O_4$ system ($x = 0, 0.2, 0.4, 0.6$) obtained via hydrothermal process using *Aloe barbadensis* Mill (Asphodelaceae) extract for the treatment of contaminated waters

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Application of iron oxide nanoparticles for removal of pollutants

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The use of iron oxide-based nanomaterials for water source pollutant removal is a relevant area of research. This study examines the effectiveness of different iron oxide-based nanomaterials in removing organic pollutants and heavy metals, specifically 2,4-dichlorophenoxyacetic acid (2,4-D) and mercury ions (Hg+2). Nanomaterials include Magnetic Activated Carbon (MAC) derived from yam residues and Functionalized Magnetic Nanoparticles (MNP) with organic ligands such as aminopropyl silane (MNP-APS), peptone (MNP-P), and yam peel biomass (MNP-YP) [1], [2]. The nanomaterials' morphology, crystalline structure, chemical groups, magnetic properties, and pollutant removal effectiveness were studied. The adsorption of Hg+2 and 2,4-

D was studied using aqueous batch systems adsorption and regeneration tests at different pH levels, initial concentrations of pollutants, and temperatures. The results show that MAC and MNP have high pollutant removal capacities in water under optimal conditions (95 mg 2,4-D/g MAC and 60 mg Hg+2/g MNP). The adsorbents' magnetic properties (6 emu/g MAC and 66 emu/ g MNP) facilitate their separation from water media, enhancing the efficiency of pollutant removal processes. It is worth noting that MAC retains 60% of its initial capacity even after undergoing five cycles of magnetic separation and regeneration. Furthermore, it investigates the green synthesis of iron oxide nanoparticles using an extract from *Cymbopogon citratus* [3]. It examines the nanoparticle's physicochemical properties and biocompatibility in which *Caenorhabditis elegans* nematodes are used as the biological model. The presence of organic molecules on green synthesis iron oxide nanoparticles promotes no toxicity and low effects on locomotion, growth, and reproduction. The biocompatibility results suggest a low risk of using these functional nanoparticles for environmental applications and an outstanding synthesis route with a green approach. These findings highlight the potential of environmentally friendly techniques in developing efficient pollutant removal strategies and functional nanomaterials for environmental applications. Combining innovative materials and sustainable approaches can pave the way for cleaner water resources and a healthier environment.

Keywords: magnetic adsorbents, pollutant removal, green synthesis

Topic: Iron Water Treatment

References

- [1] Herrera-García, U., Castillo, J., Patiño-Ruiz, D., Solano, R., & Herrera, A. Activated carbon from Yam Peels Modified with Fe₃O₄ for removal of 2,4-dichlorophenoxyacetic acid in aqueous solution. *Water*, 2019; 11.
- [2] Marimón-Bolívar, W., Tejada-Benítez, L., & Herrera, A. P. Removal of mercury (II) from water using magnetic nanoparticles coated with amino organic ligands and yam peel biomass. *Env. Nano.*, 2018; 10: 486–493.
- [3] Patiño-Ruiz, D., Sánchez-Botero, L., Tejada-Benitez, L., Hinestroza, J., & Herrera, A. Green synthesis of iron oxide nanoparticles using *Cymbopogon citratus* extract and sodium carbonate salt: Nanotoxicological considerations for potential environmental applications. *Env. Nano*, 2020; 14.

Magnetic remediators as remarkable alternatives for real water treatments: current challenges and perspectives

Magnetic remediators are novel and interesting materials to treat polluted soils and water bodies. This is due to their high catalytic response, remarkable specific surface area, pulling magnetic response, and adsorption sites [1]. The aim of this talk is to present the most optimal physicochemical conditions for removing lead from real water effluents using magnetic zeolite composites. Specifically, in the Cumbaza River located in the Department of San Martín, Peru [2]. In that sense, we will discuss the adsorption protocols developed by our research group [1,2]. Besides, novel ecotoxicological experiments to determine the lethal concentrations to apply these magnetic remediators for short-term adsorption periods in water effluents will be presented in the workshop [3]. Current challenges and perspectives representing the scale-up synthesis process and the costs of implementing this technology at the level of industries will also be discussed.

Keywords: Water conservation and sustainability; Magnetic composite; After-adsorption properties; Magnetic uptake; Ecotoxicology.

Topic: Water Treatment

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References

- [1] Ramos-Guivar J.A., Flores-Cano D.A., Passamani, E.C. Differentiating nanomaghemite and nanomagnetite and discussing their importance in arsenic and lead removal from contaminated effluents: A critical review. *Nanomaterials* 2021; 11: 1-31.
- [2] Ramos-Guivar J.A., Checca-Huaman, Noemi-Raquel, Litterst, F.J., Passamani, E.C. Synergetic effect between zeolite 5 A and maghemite nanoparticles for fast lead uptake from the Peruvian river Cumbaza: Study of surface adsorption mechanism using X-ray photoelectron spectroscopy. *Appl. Surf. Sci. Adv.* 2023; 18: 100489.
- [3] Tamanaha-Vegas C. A., Zarria-Romero J.Y., Greneche, J.-M., Passamani E.C., Ramos-Guivar J.A. Surface magnetic properties of a ternary nanocomposite and its ecotoxicological properties in *Daphnia magna*. *Adv. Powder Technol.* 2022; 33: 103395.

Retention potential of contaminants by (nano) magnetite in batch and microfluidic systems

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The scientific community has greatly focused on finding innovative remediation techniques for the decontamination of drinking and waste water. (Nano)magnetite (Fe₃O₄) has been suggested to be a significant reductant for contaminants due to its ubiquity in the environment, and its great adsorption capacity and ability to retain metals on its high specific surface [1]. Its use has become an emerging technology for

the treatment of contaminated land and water with a great potential to become an effective and low-cost alternative to conventional remediation techniques.

We have taken advantage of a concept of the circular economy, exploiting an existing waste from the steel industry that HYMAG'IN company has transformed into magnetite, to study the immobilisation of As, Sb, and U and provide new insights into a new 'green' route for the decontamination of water. The results showed up to 98% U removal under controlled pH conditions, while phosphate did not hinder this immobilization [2]. In contrast, the results confirmed the limited uptake of As and Sb oxyanions by magnetite in presence of phosphate as the competing anion [2]. To limit this wastewater problem, raw ZVI anaerobic oxidation was examined as mechanism to increase the pH and as a source of Fe²⁺ to remove phosphate via vivianite precipitation, prior to the reaction with magnetite. It is anticipated that an optimum 3-steps design with separate reactors controlling the conditions of ZVI oxidation, followed by vivianite precipitation and finally, reaction with magnetite, can achieve high contaminant uptake in field applications [2].

Polymeric coatings can also stabilize the iron oxide/hydroxide with respect to aggregation, maximizing the adsorption capacity [3]. Bionanocomposite aggregates (chitosane/PEG-magnetite) may be used to immobilize antimony in water treatment plants. We mimic those systems in a micro-scale format via the use of polymer aggregates and microfluidics to study time-dependent Sb reduction by nanomagnetite, and measure the reactive diffusion of Sb within these aggregates. Synchrotron X-ray spectroscopy and fluorescence are applied for the first time to such experimental systems to shed light into the role of nanomagnetite aggregates into Sb immobilization, as a novel remediation strategy. We show that the efficiency of the aggregate to immobilize Sb, within a 6 to 8 h residence time, depends on the Sb input concentration and oxidation state, and on the presence or not of nanoparticle coating (chitosan).

Keywords: (Nano)magnetite, Sorption processes, Remediation strategy

Topic: Water treatment

References

- [1] Missana, T., U. Alonso, A. C. Scheinost, N. Granizo, and M. García-Gutiérrez. Selenite retention by nanocrystalline magnetite: Role of adsorption, reduction and dissolution/co-precipitation processes. *Geochim. Cosmochim. Acta* 2009; 73(20): pages 6205-6217.
- [2] Papaslioti, E. M., Le Bouteiller, P., Carreira, H., Greneche, J. M., Fernandez-Martinez, A., & Charlet, L. Immobilisation of contaminants by 'green'-synthesized magnetite as a remediation approach to the phosphogypsum waste leachates model solution. *J Environ Manage* 2023; 341: page 117997.
- [3] He J., Bardelli F., Gehin A., Silvester E., and Laurent Charlet L. Novel chitosan goethite bionanocomposite beads for arsenic remediation. *Water res.* 2016; 101: pages 1-9.

Utilization of akaganeite nanoparticles for adsorption of heavy metals in water

Pasquier [2] investigated ten adsorption kinetics models, applying them to lead adsorption using activated carbon. Additionally, Valencia [3] utilized twenty-two kinetic models to fit experimental data previously documented in the literature. Adsorption kinetics not only provide insights into the rate of contaminant removal when utilizing adsorbents, a critical parameter for designing and operating efficient adsorption systems [3], but also offer an indication of the nature of the interaction involved in the reaction. This provides valuable insights for the potential utilization of the material in upcoming experimental applications [1].

This research aims to compare the adsorption capacities of pure akaganeite with various heavy metals, employing different models of adsorption kinetics documented in the existing literature.

Keywords: adsorption kinetics, akaganeite, water contaminants
Topic: Water Treatment

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Akaganeite, with the chemical formula β -FeOOH, has been employed as an adsorbent for treating polluted water to eliminate various toxic ions. This is attributed to its ion exchange capacity facilitated by structural chlorine, the presence of tunnels, and its extensive irregular surface [1].

Akaganeite has been utilized in numerous studies as an adsorbent for various substances. For example, Largitte and

References

- [1] V. Villacorta et al. RSC Adv., 2020,10: pages 42688-42698.
- [2] L. Largitte and R. Pasquier. 2016. ChERD 109: pages 495-504.
- [3] A. Valencia Álvarez. 2022. Cinéticas de adsorción de contaminantes en medios acuosos usando adsorbentes basados en óxidos de hierro. Trabajo de grado para optar al título de Físico. Facultad de Ciencias Exactas y Naturales. Universidad de Antioquia. Medellín.

Magnetic iron-based nanoadsorbents for boron and phosphorus remediation

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Boron (B) and phosphorus (P), either as ions or in compounds, are, in general, essential nutrients for agriculture. However, when their presence exceed the permitted level in the water (contaminated effluents), they cause environmental damage by directly or indirectly affecting living organisms and plants [1]. Sources of P and B contamination are diverse, including sewage wastewater, detergents, fertilizers, and others. In recent years, magnetic remediation has emerged as a suitable method for water treatment. However, magnetic adsorbents must be developed and deeply studied first in a controlled effluent (synthetic), before the application in the multicomponent effluents found in nature. In this presentation, we will discuss a set of functionalized magnetic iron-oxide adsorbents for application in B and P remediation. Our Fe-oxide-based nanoadsorbents were synthesized using the co-precipitation method and carefully characterized by X-ray diffractometry, infrared and ⁵⁷Fe Mössbauer spectroscopies, nuclear magnetic resonance, magnetization, electron microscopy (both transmission and scanning), and surface area analysis to comprehend their structural, morphological, hyperfine, and magnetic properties before and after P or B adsorptions. The magnetic nanoadsorbents are nanoparticles of maghemite (γ -Fe₂O₃) or Mg-ferrite (MgFe₂O₄) functionalized with MgO, with the former phase responsible for magnetic properties, whereas the latter one is responsible for the P or B removal process. Kinetics and isothermal models were applied to describe the types of adsorption processes that have occurred between B- or P-species and Mg-rich phases.

Keywords: ⁵⁷Fe Mössbauer spectroscopy, Hyperfine Interactions, Fe-oxides, magnetic remediation, boron and phosphorus removal.

Topic: Water treatment

References

World Health Organization (2022) Guidelines for drinking-water quality, 4th edition, incorporating the 1st addendum. <https://www.who.int/publications-detail-redirect/9789241549950>. Accessed 26 Apr 2022.

Synthesis and characterization of nanocrystalline ferrites from the $Mn_{1-x}Zn_xFe_2O_4$ system ($x = 0, 0.2, 0.4, 0.6$) obtained via hydrothermal process using Aloe barbadensis Mill (Asphodelaceae) extract for the treatment of contaminated waters

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The synthesis of nanocrystalline spinel ferrites has become an important part of novel materials research. The study of these materials has great relevance in modern technological applications in various industrial and biological fields [1]. It is well known that the preparation method can strongly affect the composition and microstructure of spinel-type nanocrystalline ferrites, and therefore, their chemical, structural and magnetic properties. Among the existing physical and chemical methods for the synthesis of spinel nanocrystalline ferrites, as high energy mechanical alloy [2], sol-gel method, polyol process,

co-precipitation method, solid state reaction method, auto-combustion method, ceramic processing method [3]. However, recent research has reported the synthesis of spinel nanoferrites via hydrothermal, using eco-friendly solvents from plant extract.

In this work, the MnZn nanocrystalline ferrites were synthesized by the hydrothermal method, the $Mn_{1-x}Zn_xFe_2O_4$ ($x=0, 0.2, 0.4, \text{ and } 0.6$) system varying the compositions of Mn and Zn, using the extract of the aloe barbadensis mill plant as a solvent environmental friendly. The influence of the composition on the morphology, microstructure and its optics properties of the final product obtained were studied through the characterization of the samples by X-Ray Diffraction (XRD), Scanning Electron microscopy (SEM), Transmission Electron Microscopy (TEM) and UV visible spectroscopy (UV-VIS). It will be evaluated which of the compositions of the Mn – Zn system is the most effective for the treatment of water contaminated with dyes. The ferrite powders obtained were spinel phase, with secondary phases (hematite) except for $x = 0.6$, the synthesized Mn-Zn ferrite had the best performance, which was a pure spinel-type crystalline structure. The average crystallite size, estimated from Scherrer equation, the size was on the order of nanometers. For SEM and TEM, it was observed that the ferrites are agglomerated, and their structure is quasispherical. The UV-Vis spectroscopy determines the direct energy bandgap which increases from ~ 2.47 to ~ 2.57 eV.

Keywords: nanocrystalline ferrites, hydrothermal, XRD, SEM, TEM UV-Vis.

References

- [1] Sharma I and Garg E. A Review on Nanoferrites in Biomedical Applications. IJBAS. 2022; volume 11: pages 1-4.
- [2] Younes A. Kherrouba N, Bouamer A. Magnetic, optical, structural and thermal properties of copperferrite nanostructured synthesized by mechanical alloying. MNA2 2021; Volume16: Pages 251-256
- [3] Preeti T, Deepika C, Shilpa T, Nikhil B, Atul T. A review on MnZn ferrites: Synthesis, characterization and applications. J Ceramint 2020 Volume 46: Pages 15740-15763.

Iron Oxide Workshop: Energy and Environment

Conferences

A geological perspective of plastic pollution

Prof. Nelson Rangel

(Uniatlantico, Colombia)

Nanomaterials for applications in energy, environment, and medicine: Advances and challenges in Latin America for the contribution to the Sustainable Development Goals

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A geological perspective of plastic pollution

This cycle reveals the transformation of plastics into new forms of pollution characteristic of the Anthropocene. With 91 % of discarded plastics never recycled, they accumulate in the environment and enter the geological record through processes like photodegradation, thermal stress, and biodegradation. The proposed Plasticene stage within the Anthropocene is defined by the post-World War II surge in plastic production and their incorporation into sedimentary processes and rocks. The study of plastics in the geologic record serves as a warning of their negative impacts and highlights the urgency of addressing plastic pollution for a sustainable future.

Keywords: Anthropocene; Litter; Plastic Geological Cycle.

Topic: Anthropocene

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The Anthropocene, the most recent geologic time division, marks humanity's profound impact on Earth. Amidst debates, the Anthropocene Working Group recommended its inclusion in the International Chronostratigraphic Chart (ICC). This period is characterized by the mid-20th century Great Acceleration Event Array (GAEA), which includes widespread presence of pollutants such as radionuclides, organochlorine pesticides, PCBs, and plastic production. The Anthropocene concept should raise public awareness of these threats, with plastic pollution being a primary concern. Plastics are now pervasive and serve as a marker for the Anthropocene Epoch or Age. Understanding their entry into the geological record requires considering the "Plastic Geological Cycle," which encompasses extraction, production, use, disposal, degradation, fragmentation, accumulation, and lithification.

Nanomaterials for applications in energy, environment, and medicine: Advances and challenges in Latin America for the contribution to the Sustainable Development Goals

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Nanoscience and nanotechnology have shown their potential to contribute to the energy transition and overcoming socio-environmental and health problems. In Latin America, progress has been made in the production of new knowledge in the field, but there are obstacles to taking advantage of it in the generation of innovations for the benefit of the populations most affected by such problems and challenges [1]. This work combines bibliometric approaches, social network analysis and case studies, to address the following question: How does the knowledge generated in Latin America about nanomaterials applied to energy, environment and medicine contribute to the achievement of the Sustainable Development Goals?

Based on data from scientific publications, patents and documentation on projects related to the topics of interest, an analysis is carried out from the transformative innovation approach [2]. The results show the existing networks and the advances and challenges to enhance the application of developments in nanomaterials.

References

- [1] Invernizzi, N., Foladori, G., Robles-Belmont, E., Záyago Lau, E., Figueroa, E. A., Bagattolli, C., Carrozza, T. J., Chiancone, A., & Urquijo, W. (2015). Nanotechnology for social needs: Contributions from Latin American research in the areas of health, energy and water. *Journal of Nanoparticle Research*, 17(5), 233. <https://doi.org/10.1007/s11051-015-3037-y>
- [2] Romero Goyeneche, O. Y., Ramirez, M., Schot, J., & Arroyave, F. (2022). Mobilizing the transformative power of research for achieving the Sustainable Development Goals. *Research Policy*, 51(10), 104589. <https://doi.org/10.1016/j.respol.2022.104589>



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