CONTRATOS PREDOCTORALES 2020 SEVERO OCHOA

PROJECT TITLE / JOB POSITION TITLE:

Development of new polar oxynitrides

RESEARCH PROJECT / RESEARCH GROUP DESCRIPTION:
(2.000 characters – including spaces)

The substitution of the anion O^{2-} by N^{3-} expands the properties of metal oxides, and oxynitrides are an emerging group of materials showing colossal magnetoresistance, visible light-active photocatalytic activity and large permittivity among other important properties. (1-5) Nitrogen and oxygen show similar electronic and crystal chemistry features, and may substitute for each other in the same crystallographic sites. Nitrogen is less electronegative, more polarizable and more charged than oxygen, increasing the covalent character of the bonds, the band gap and the crystal field splitting, hence the design of transition metal oxynitrides is a suitable strategy to look for new electronic properties.

The project of this doctoral thesis aims at the search of new oxynitrides of transition metals with distorted environments and ordering of anions that may lead to long-range ordered electrical dipoles and ferroelectricity. Nitride stabilizes high oxidation states of the cations, that may suffer distortions caused by electronic effects such as second order Jahn-Teller, enhanced by N/O order and by electrostatic repulsions. An example of success of this strategy is the non-centrosymmetric polar oxynitride $BaWON_2$ that we have recently discovered (see J. Oró-Solé, J. Fontcuberta, A. Fuertes et al, Angew. Chem. Int. Ed. 2020, 59, 18395–18399). It is a hexagonal perovskite that shows total order of oxygen and nitrogen in highly distorted W^{6+} octahedra. The present project will develop chemical modifications of this compound as well as other oxynitrides with different structures susceptible to show long-range ordered electrical dipoles and spontaneous polarization.

References: (1) M. Yang, A.Fuertes, J.P.Attfield et al, J. Am. Chem. Soc. 132 (2010), 4822. (2) M.Yang, A.Fuertes, J.P.Attfield et al , Nature Chem. 3 (2011), 47. (3) A.Fuertes, Mater. Hor. 2 (2015), 453. (4) C.Frontera, A.Fuertes et al, Chem. Comm., 52 (2016), 4317. (5) R.Ceravola, A.Fuertes et al, Chem. Comm. 55 (2019), 3105.

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JOB POSITION DESCRIPTION:
(2.000 characters – including spaces)
Include all the relevant information about the position, role, responsibilities and skills required within the project/group

Oxynitrides containing alkaline earth or rare earth cations and transition metals will be designed and developed to produce the new electronic materials. The student will be trained in non-conventional synthetic methods at high temperatures with strict control of atmosphere and other parameters in order to produce the targeted oxynitrides. The student will perform the preparation of powder samples at high temperatures in nitriding atmospheres as well as the characterization of the chemical composition, crystal structure and physical properties. The investigation of the crystal structure will be performed by using X-ray diffraction, transmission electron microscopy and electron diffraction at ICMAB, and also at international facilities like the ALBA synchrotron and neutron diffraction (Institut Laue Langevin in France). The electronic properties of the oxynitrides will be studied by magnetization and electrical measurements as a function of temperature and magnetic field. The crystal structure will be determined by using the Rietveld method from powder diffraction data and the structural parameters will be correlated with the observed physical properties.

Expected academic requirements and skills required for the position:

- Degree in Chemistry or Materials Science
- Academic grades will be considered in the evaluation
- Research experience will be considered in the evaluation
- High motivation for experimental research
- Working aptitudes in a collaborative group
- High level in written/spoken English

GROUP LEADER:

Title: Prof.
Full name: Amparo Fuertes
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Research project / Research Group website: Engineering complex inorganic materials for energy applications (ECIME) (Reference: PID2020-113805GB-I00)
http://departments.icmab.es/ssc/nitride-based-materials/

RELATED LINKS TO THE POSITION (optional)
URL: https://departments.icmab.es/ssc/nitride-based-materials/
Tittle link: Research on nitride materials at ICMAB

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