OFERTA DE PROYECTO DE TESIS DOCTORAL AYUDAS PARA LA FORMACIÓN DE PROFESORADO UNIVERSITARIO (FPU) 2018

APELIDOS Y NOMBRE DEL DIRECTOR
Amparo Fuertes, Miquel

TITULO DE LA TESIS
Perovskite oxynitrides with new electronic properties

AREA CIENTIFICA
Ciencia y Tecnología de Materiales

CENTRO/INSTITUTO
Instituto de Ciencia de Materiales de Barcelona (ICMAB)

COMUNIDAD AUTONOMA/PROVINCIA
Cataluña

CORREO ELECTRONICO DEL DIRECTOR
amparo.fuertes@icmab.es

WEBSITE GRUPO DE INVESTIGACION O CENTRO/INSTITUTO
http://departments.icmab.es/ssc/nitride-based-materials/
The project of this doctoral thesis aims at the development of perovskite oxynitrides as new electronic materials with magnetic, dielectric or colossal magnetoresistance properties. Transition metal oxides show important physical properties including colossal magnetoresistance, high temperature superconductivity and ferroelectricity. The partial substitution of the anion oxide by nitride expands and tunes their physical properties, and oxynitrides are an emerging group of solids where the oxidation states of the transition metal, bond covalency, bond polarization and band gaps are modified by nitride. 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 and its introduction in an oxidic compound increases the covalent character of the bonds with the cations and the crystal field splitting. This results in changes in the electronic levels that affect the physical properties. The higher charge of nitride (-3) versus oxide (-2) allows the design of perovskites with high oxidation states of the transition metals increasing the polarization and changing the magnetic properties and the conductivity with respect to oxides. The research group hosting the student has a long experience in the development of new nitrided materials with a diversity of properties including superconductivity, photocatalytic water splitting, colossal magnetoresistance and luminescence.

Perovskite oxynitrides will be developed to produce new electronic materials containing lanthanides and late transition metals as magnetic cations. 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 the Institute of Materials Science of Barcelona, and also at international facilities like the ALBA synchrotron and neutron diffraction (Institut Laue Langevin in France or ISIS in UK). The electronic properties of the perovskite oxynitrides will be studied by magnetization and electrical resistivity 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.