

ADDITIONAL INFORMATION

The recruited PhD researcher will not only familiarize with a wide range of different synthesis strategies applied to non-oxide compounds but also with a wide variety of complementary characterization techniques and the assessment of their performance in energy related applications. He/she will have office space with a computer and bench space within the lab, and also access to all the facilities at ICMAB including equipment and scientific services. The ICMAB is multicultural and multidisciplinary, with researchers from many different countries, which will provide a very diverse environment for research, offering also the opportunity to interact and learn from other researchers with extensive expertise and background in a wide array of scientific fields. The supervisors will keep a weekly track of the progress through scheduled meetings to ensure proper support and guidance during the PhD and she/he will have the opportunity to present research progress during fortnightly group meetings, held in English, which will allow improving communication skills. ICMAB offers a complementary training program in Functional Materials including soft, transversal, interdisciplinary and specific skills. It includes training in research planning and execution; hands-on in experimental techniques at ICMAB Scientific Equipment Platforms, fortnightly top-level international scientific seminars and annual technical workshops. Thematic workshops that are also periodically organized at ICMAB dedicated to characterization techniques (which are available as facilities to which the PhD will have access) will also be of paramount importance.

The PhD student will be enrolled in the Materials Science PhD program from Universitat Autònoma de Barcelona, which involves the departments of Physics, Chemistry and Geology and has been awarded the Excellent Accreditation seal by the Catalan Quality Agency (AQU). The objective of this program is to offer students the tools and knowledge to be able to undertake and complete an original and innovative research project and a personalized Career Development Plan will be defined together with the supervisors including (i) details on the scientific project, (ii) the timeline of training, (iii) secondments to other institutions, (iv) potential contacts with industrial partners, (v) list of skills to be obtained during training, (vi) activities tracking, (vii) objectives monitoring and (viii) quality assessment. The career development plan will be designed by the supervisors together with the PhD student and continuously monitored within ICMAB's mentoring program. The PhD student and the mentor (permanent scientific staff from a different ICMAB Research Unit) will formally meet every three months and additional informal meetings will take place as often as needed. The task of the mentor will be guiding the student with all issues that go beyond the scientific day-to-day of the PhD Thesis. These include, but are not limited to (i) relation with the supervisors and quality of the supervision received; (ii) monitoring of the PhD Thesis progresses; (iii) monitoring of the career development plan; (iv) professional future career orientation (academic and industrial possibilities).

For the PhD project of the student two secondments are planned in worldwide recognized laboratories. A two-month stay is planned at the University of Kyoto (Japan), under the supervision of Prof. Ryu Abe with whom the proposing group has been collaborating since 2016 and a one-month stay could be scheduled at Oxford University under the supervision of Dr. Theodosios Famprikis, who has a very strong track record in the study of lithium ionic conductors (including nitride based fully reduced systems).

The student will be offered the possibility to deliver oral presentations or posters at national or international conferences (normally a minimum of one conference per year), which will improve

the communication skills. A minimum of two scientific papers are expected to be produced from the PhD specific research within the UAB Materials Science PhD program, the average number of publications for previous PhD students in the group is 7.2 articles, 61% of them as first author.

SUMMARY OF SUPERVISORS CV

Prof. Amparo Fuertes (ORCID ID 0000-0001-5338-9724)

She started her research career at the University of Valencia where she developed a PhD thesis on the study of magnetic transition metal carboxylates with interactions of low dimensionality. On 1986 she was appointed as a postdoctoral researcher at the crystallography group of the Institute Jaume Almera (CSIC), Barcelona, and she was awarded the Ibero-American Crystallography Prize by the National Commission of 5th Centennial of the Discovery of America and the Institute of Ibero-American Cooperation. On 1988 he was appointed as tenured scientist of CSIC at the Institute of Materials Science of Barcelona (ICMAB) where she started and directed the Solid State Chemistry Laboratory. From 2006 she is a research professor of CSIC, and head of the Department of Solid State Chemistry until 2023. In 2008-2009 she was an invited professor at the School of Chemistry at the University of Edinburgh (UK). From 2009 to 2016 she was deputy president of the specialized group of Solid State Chemistry of the Spanish Royal Society of Chemistry. Since 2022 she is a member of the Spanish National Committee for Crystallography that represents Spain in the International Union of Crystallography. She has developed research in the fields of low dimensional molecular transition metal compounds, superconducting and nitride materials.

She has published 132 articles included in Web of Science being corresponding author in 42 % of total articles and in 75 % of articles in last 10 years. These have been referenced 3152 times with h-index= 31. She is included in the 2023 top 2 % scientist list of the Stanford University. Her present research focusses on the synthesis, structure and properties of metal nitrides and oxynitrides with applications as photocatalysts, battery materials, phosphors, magnetic materials, superconducting and dielectric materials. Selected research articles in this field as main author are: 1) Engineering Polar Oxynitrides: Hexagonal Perovskite BaWO_2 . *Angew. Chem. Int. Ed.* 59, 18395 (2020). 9 citations. 2) Anion Order in Perovskite Oxynitrides. *Nat. Chem.*, 3, 47 (2011). 207 citations. 3) Electronic Tuning of Two Metals and Colossal Magnetoresistances in $\text{EuWO}_{1+x}\text{N}_2$ -x Perovskites. *J. Am. Chem. Soc.*, 132, 4822 (2010). 91 citations. 4) Large Coupled Magnetoresponses in EuNbO_2N . *J. Am. Chem. Soc.*, 130, 12572 (2008). 92 citations. 5) Nitrogen Doping of Ceria. *Chem. Mat.* 20, 1682 (2008). 61 citations. 6) Prediction of Anion Distributions using Paulings Second Rule. *Inorg. Chem.*, 45, 9640 (2006). 60 citations.

She is periodically invited to give keynote talks in international conferences in the field of materials chemistry (27 talks in last 10 years) and to submit articles in important journals of the area (7 papers in last 10 years). Invited perspectives: *Dalton Trans.* 2010(94 citations), *J. Mat. Chem.* 2012(166 citations), *Sem. Sci. Tech.* 2014, *Materials Horizons* 2015(130 citations), *Prog. Sol. State Chem.* 2018(34 citations), *APL Mat.* 2020(25 citations). Chair of National/International Conferences. Member of the Advisory Board of *Journal of Materials Chemistry* (2010-2012) and *Journal of Materials Chemistry A* (2013-2014), and Regional European Editor of *Solid State Sciences*(Elsevier)(2022-).

She has been principal investigator of AEAT projects including most recent PID2020-113805GB-I00, MAT2017-86616-R, MAT2014-53500-R and MAT2011-24757, and several projects of Solid State Chemistry group funded by the Generalitat de Catalunya.

Prof. M. Rosa Palacín (ORCID ID 0000-0001-7351-2005)

Her scientific activity initiated in 1995 after completion of PhD on solid state chemistry dealing with complex perovskite oxides (UAB) at ICMAB-CSIC. Following a post-doctoral stay at LRCS (France), she started a research line on inorganic battery materials at ICMAB-CSIC in 1998.

Her career has been fully focused in solid state chemistry (synthesis and crystal chemistry) and electrochemistry applied to batteries and covered a wide diversity of technologies with either aqueous or organic electrolytes. These include already commercial (e.g. Ni or Li-ion) or pre-commercial (Na-ion) concepts, as well as new emerging chemistries such as those based on Mg or Ca, in which she has been pioneer. Her main accomplishments include (i) understanding of the structural transformations taking place at the positive electrode in Ni based batteries through *operando* diffraction and correlation between defects in the crystal structure and electrochemical performance, (ii) systematization of mechanisms and bottlenecks in electrode materials operating via conversion redox reactions in lithium cells, (iii) pioneering electrolyte optimization for Na-ion batteries and (iv) demonstration of the viability of calcium metal as anode material, first step towards proof-of-concept of a new calcium based rechargeable battery technology. Her sustained interaction with industry either through direct research contracts or diverse institutional/reviewing appointments has enabled a practical perspective in terms of sustainability, cost, etc. which has been extremely valuable to orient her research. She has always placed emphasis on developing fertile cooperation scenarios between basic oriented research and industry, and often performed research under direct industrial contracts.

She has published > 160 articles in peer reviewed journals, referenced over 14000 times and is included in the 2023 top 2 % scientist list of the Stanford University. She is co-inventor in 10 patents (6 of them jointly owned with industry) and PI of 4 National and 8 European competitive grants and 5 multi-annual industrially funded projects, always related to battery research. Her achievements have led to the establishment of a significant number of collaborations and international recognition (23 Invited/Keynote talks in the last 5 years), being also invited to write reviews in both high impact and specialized journals. These cover materials (standard or new redox concepts, aqueous and non-aqueous technologies) and also degradation/failure mechanisms with those in Chem. Rev. (2020, 193 cit.), Chem. Soc. Rev. (2009, 1261 cit. and 2018, 142 cit.), Science (2016, 608 cit.), JACS (2015, 456 cit.), JES (2015, 491 cit.) and Adv. Mat. (2010, 2180 cit.) deserving special mention.

She serves as an associate editor for Chemistry of Materials (ACS) and was elected to the Governing Board of Batteries Europe ETIP in 2019. In 2021 she was appointed as Fellow of the Electrochemical Society and received the Research Award from the International Battery Association. She has also been awarded the Spanish-French Miguel Catalán - Paul Sabatier prize by the French Chemical Society, delivered in June 2023.