

CONTRATOS PREDOCTORALES – MATRANS24 (CEX2023-001263-S)

RESEARCH CHALLENGE:

Emerging functionalities in curved materials

PROJECT TITLE / JOB POSITION TITLE:

Curvature Induced Magnetic and Spin-Orbit Couplings from first principles

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

In this project, we aim at exploring new strain-gradient (curvature) effects on the electrical and magnetic properties of materials, and at developing appropriate theoretical and methodological tools to facilitate their computational study. The primary focus will be on understanding how curvature, by breaking space inversion (SI) symmetry within the bent layer, allows for the emergence of physical properties that are absent in the unstrained sample.

A paradigmatic manifestation of SI breaking in a conductor is the intrinsic spin-Hall effect. This phenomenon is commonly ascribed to the Rashba coupling, which is larger in systems with a sizeable electric polarization and a strong spin-orbit coupling. Unfortunately, existing materials that display these characteristics "out of the box" are scarce. Here, we shall explore curvature as a universal route to engineering a Rashba effect in any material via mechanical means, with special focus on two-dimensional systems.

Strain gradients can have a comparably strong impact on magnetism, via a curvature-induced modification ("flexomagnetism") of the spin coupling parameters. To cope with the impressive experimental advances in this area, an adequate theoretical support is essential. Quantitative first-principles approaches are ideally suited to attack this problem, but the existing methodologies are still inadequate: In this project, we shall build on recent advances in the context of flexoelectricity to establish a comprehensive theoretical framework.

The PIs of the PhD project are ideally suited to supervise this activity. They are both worldwide leaders in the first-principles theory of flexoelectricity and flexomagnetism, of which they have been the most prominent developers over the past 10 years. They have authored the state-of-the-art public code implementation of the methodologies to treat strain gradients [www.abinit.org], and applied it to several types of materials, ranging from perovskite oxides, two-dimensional crystals and polar metals.



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JOB POSITION DESCRIPTION:

(Max. 2.000 characters – including spaces)

Include all the relevant information about the position, role, responsibilities and skills required within the project/group

We expect the candidate to carry out first-principles calculations within the framework of density-functional theory, with an emphasis on linear-response perturbative techniques. The candidate will be encouraged to acquire a deep knowledge of the underlying theory and algorithms, and to develop novel computational tools on top of the existing ones. Given the challenging nature of this project, we welcome applications from especially skilled individuals, with a genuine interest in building a solid knowledge of fundamental condensed-matter physics. The Theory and Simulation group at ICMAB is an excellent environment to carry out frontier research in first-principles methods and applications. MS and MR have a strong record of successfully training young researchers on the fundamentals, of guiding them in innovative directions, and of maximizing the public recognition of their early-career work.

The PhD student will enroll in the Doctoral Program in Physics (<https://www.uab.cat/en/phds/physics>) at the Universidad Autònoma de Barcelona (UAB). The Physics Department of UAB is a frequent partner of our research group and provides ideal support for the training needs and career planning of the student. As part of the program, students are encouraged to take a three-months secondment stay at a foreign research institution; most of our students have chosen to visit our long-term US collaborators (David Vanderbilt at Rutgers University, and Cyrus Dreyer at Stony Brook and Simons Foundation), which are ideal destinations both in terms of scientific environment and international prestige. Our students are also strongly encouraged to travel to international conferences and workshops as often as possible, to maximize visibility for their activity and start building a professional network early on.

PhD CO-DIRECTORS:

Prof./Dr: Massimiliano Stengel

Email: mstengel@icmab.es

Research group website: <https://icmab.es/ts/leem>

Prof./Dr: Miquel Royo Valls

Email: mroyo@icmab.es

Research group website: <https://icmab.es/ts/leem>

RELATED LINKS TO THE POSITION (optional)

URL:

Title link: