PhD Project

Theoretical studies of orbitronic and spin-orbit phenomena in heterostructures comprising van der Waals materials, metals and oxides

Contacts : M. Chshiev (Spintec) and J. Li (Leti)

The rapid development of information technologies requires the processing and storage of huge quantities of digital data that continues to grow exponentially over the years, leading to a dramatic increase in energy consumption and storage capacity requirements. Spin electronics, or spintronics, can help meet these challenges, as it is a dynamic field, rich in innovative applications and fundamental physical phenomena that gives rise to novel development of industrial applications in the fields of magnetic recording, sensors and memory devices. Spin-orbit phenomena such as perpendicular magnetic anisotropy (PMA) or Dzyaloshinskii-Moriya interaction (DMI) have become of tremendous interest since they play a major role in particular for magnetic random access memories based on spin transfer (STT-MRAM) and spin-orbit torques (SOT-MRAM) as well as in emergence of spin-orbitronics[1,2,3]. At the same time, 2D materials such as graphene, transition metal dichalcogenides and associated van der Waals heterostructures including 2D magnets have become of major interest in recent years since they may serve as efficient alternatives for these and next generation of spintronic devices, thus giving rise to emergence of graphene and 2D spintronics[4,5,6]. Finally, a fascinating new field of research has been emerging very recently called orbitronics[7] that exploits orbital currents instead of spin currents in spintronics and spin-orbitronics.

The proposed PhD thesis will provide multi-scale numerical calculations to find the best-unexplored combinations of transition metals, oxides and 2D materials (transition metal dichalcogenides, 2D magnets, graphene…), to design magnetic nanostructures for spintronics and emerging fields of spin-orbitronics and, very recently, orbitronics. Using ab initio calculations combined with linear response based on tight-binding approach, we will screen their potential not only for spin-orbit phenomena such as DMI, PMA and spin-charge interconversion based on Rashba and Rashba-Edelstein effects, but also focus on Orbital Rashba Edelstein Effect (OREE). Furthermore, the mechanisms of control of these phenomena via external stimuli (strain, external electric and magnetic fields) and possibility of inducing chiral magnetic structures such as skyrmions will be investigated as well. The main goal of this work will be helping finding optimal material combination to tune DMI, PMA and spin-charge interconversion efficiency to help optimizing spintronic devices making thereby a significant contribution to the development of sustainable microelectronics by proposing new generations of spin electronics applications.

The calculations will be performed on Spintec computational cluster nodes using first-principles packages based on density functional theory (DFT) combined with other simulation techniques. Results obtained will be carefully analyzed with the possibility of publication in international scientific journals. Strong collaboration with labs in France (Laboratoire Albert Fert, Aix-Marseille Univ, L2C…) and abroad (ICN2/Spain, EPFL and PSI/Switzerland…) are previewed.

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