PhD Proposal 2017

School: CS	
Laboratory: SPMS	**Web site: spms.ecp.fr**
Team: Advanced Ferroics	**Head of the team: B. Dkhil**
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Collaboration with other partner during this PhD: **In France: several groups**	**In China: XJ Meng, Shangai Institute of Physics**

Title: Looking for novel photoferroic materials
Scientific field: Materials science
Key words: ferroelectric, photovoltaic

Background, Context:

Among solar energy technologies, the most famous one is the photovoltaic which allows conversion of sunlight into electric current. While solar energy is an auspicious long-term solution for conversion in other energy forms, the modest efficiency limited by the use of semiconductor materials, plagues solar energy converters. Given the growing demand for renewable energy sources a growing interest in new pathways including new type of materials is thus highly desired. It is in this framework that this thesis project is proposed by exploring the use of ferroelectric materials to reach a next generation of photovoltaics. Ferroelectrics are materials characterized by a switchable spontaneous electric polarization. The research in ferroelectric field has been punctuated in the

recent years by the discovery of many original and novel physical phenomena. In turn, these discoveries have lead to completely new branches of materials science arising from the field of ferroelectrics and that are now massively investigated such as the ferroelectric tunnel junctions that exploit the polarization switchability in ultra-thin ferroelectric films, the ferroelectric-based piezoelectricity where the electrical polarization couples strongly with elastic strain or the field of multiferroics in which polarization and magnetism coexist simultaneously.

Most recently, we reviewed [1] the current status for these last 6 years on the emerging and fast progressing new field namely photovoltaic ferroelectrics. We identify the critical factors that need to be further explored and challenged, both experimentally and theoretically, in order to achieve a better fundamental understanding as well as higher-efficiency. This includes the role of domain walls, the ways to tune the band gap, the consequences arising from the polarization switchability, the role of defects and contact electrodes as well as the effect of downscaling. Beyond photovoltaics, other related processes like photostriction [2,3] or photocatalysis [4] are also described.

Research subject, work plan:

The main research objective of this thesis work is to better understand the physical mechanism behind the photovoltaic effect in ferroelectrics. As a matter of fact, the PhD student will study new ferroelectrics by looking for reduction of the band gap (to fit the solar spectrum) by keeping large enough polarization. Some guidelines have been already identified and will be explored such as the insertion of absorption bands within the band gap using dopant, the enhancement of the mobility by selecting the structure constituents, ...

The PhD student will join a team having already a strong and internationally recognized expertise in the field of ferroelectrics having a wide set of tools aiming a deep investigation of such materials. He/she will synthesize the samples (ceramics, thin films, …) and characterize the physical properties (dielectric constant, I-V measurements, band-gap, …) in relationship with the structure (X-ray diffraction, UV-Visible Raman spectroscopy, Piezoforce microscopy, High resolution electron microscopy, photoelectron spectroscopy, …). Depending on his/her interest the candidate could be involved in calculation using state-of-the-art modelling techniques.

The thesis work will be done at SPMS at CentraleSupélec, Université Paris-Saclay, nearby Paris, and will benefit of various national and international collaborations.

References:

[1]: C. Paillard, X. Bai, IC. Infante, M. Guennou, G. Geneste, M. Alexe, J. Kreisel, B. Dkhil
Photovoltaic with ferroelectrics: Current status and beyond
Adv. Mater. **28**, 5153 (2016)
[2]: C. Paillard, X. Bin, B. Dkhil, G. Geneste, L. Bellaiche
Photostriction in ferroelectrics from Density Functional Theory
Phys. Rev. Lett. **116**, 247401 (2016)
[3]: M. Lejman, G. Vaudel, I. C. Infante, I. Chaban, T. Pezeril, M. Edely, G. F. Nataf, M. Guennou, J. Kreisel, V. E. Gusev, B. Dkhil, P. Ruello
Ultrafast acousto-optic mode conversion in optically birefringent ferroelectcrics
Nature Comm. **7**, 12345 (2016)
[4]: Size Effect on Optical and Photocatalytic Properties in BiFeO3 Nanoparticles
X. Bai, J. Wei, B. Tian, Y. Liu, T. Reiss, N. Guiblin, P. Gemeiner, B. Dkhil, I.C. Infante
J. Phys. Chem. C **120**, 3595 (2016)