Post-Doc profile at UMφ CNRS-Thales (2023-2026)

ANR DYNTOP Project:

Spin Dynamics and non-linear effects in Magnetic Topological Insulator

The discovery of metallic quantum states at the surface of 3D topological insulators has opened exciting new functionalities in spintronics owing to their topological protection. In these quantum materials including heterostructures, the combination of band inversion and time reversal symmetry (**TRS**) results in a peculiar spin texture in momentum space: the spin-momentum locking or **SML** like recently observed by Spin and Angular-Resolved PhotoEmission or **spin-ARPES** in the case of $Bi_{1-x}Sb_x$ alloys (*Fig.1*) **[1-2].** The benefit is the generation of an out of equilibrium spin density (also called spin-accumulation) along the specific transverse direction to the in-plane injected current. This is the Rashba-Edelstein effect (**REE**) which can be used to promote spin-charge conversion (**SCC**) and spin-orbit torque (**SOT**) onto the magnetization vector of an adjacent ferromagnet (**FM**). The reciprocal phenomenon by which a spin density produces an in-plane transverse charge current is called the Inverse Rashba-Edelstein effect (**IREE**). This was recently demonstrated by the emission of electromagnetic wave in the THz range by THz-TDS emission spectroscopy for $Bi_{1-x}Sb_x$ (*Fig.1 inset*) **[2].** It has been demonstrated in a range of Bi-based TI compounds, including bismuth selenide Bi_2Se_3, bismuth telluride Bi_2Te_3, $Bi_2(Se,Te)_3$ **[3]** or $Bi_{1-x}Sb_x$ (BiSb) **[2].** To fully benefit from IREE, the charge currents should be confined in the topological surface states and any current flowing through the bulk states should be avoided. The prerequisites a sizeable bandgap (typically larger than 0.2 to 0.3 eV) together with a perfect control of the Fermi level position, usually achieved by stoichiometry and/or strain engineering. In this respect, although presenting a modest bulk bandgap (about 40 meV for x=0.07) and relatively complex band structure Bi_{1-x} Sb_x appears a very good candidate. Indeed, quantization effects in ultrathin films leads to much larger gap while retaining their band inversion near the M point in the x=0.07-0.3 composition range **[1].**

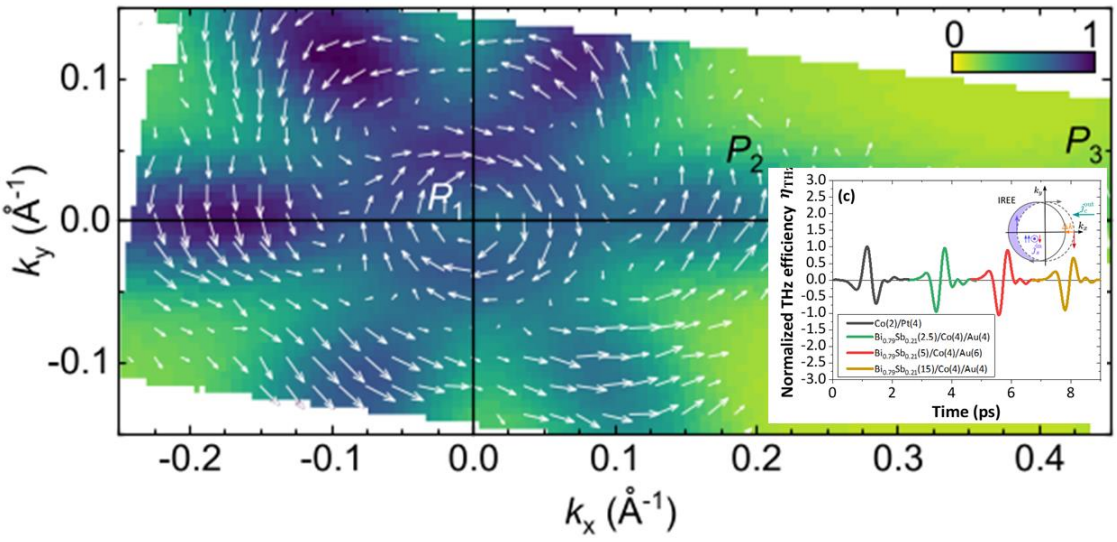

FiG.1: Scheme illustrating the spin-momentum locking measured by SARPES and subsequent ultrafast spin-charge conversion probed by THz-TDS methods in the ultrafast time domain.

For those goals, from an experimental side, two typical structures will be examined in the **ANR DYNTOP project**: *i*) the FM/TI bilayer and interfaces as previously investigated (as $Bi_{1-x}Sb_x$ and Co/ $Bi_{1-x}Sb_x$) and *ii*) magnetic topological insulators as ordered Mn-doped compounds ($MnSb_2Te_4$) or disordered Cr-doped compounds ($Bi_{2-x}Cr_xSe_3$, $Sn_{1-x}Cr_xTe$). Finally, taking benefit of our previous work, we will study heterostructures as MTI/TI ($Bi_{2-x}Cr_xSe_3/Bi_2Se_3$) or FM/TI ($Cr_2Te_3/Bi_2Te_3$). Both theoretically and experimentally, these materials are known to be 3D time-reversal symmetric TI **[4-5].** The topologically non-trivial band structure of this material arises from relatively strong spin-orbit coupling, which causes a band inversion at the Γ point.

In this project, we want to address **two major research axes**: (1) the dynamics and relaxation mechanism of carriers and spins in bulk and at the surface as well as (2) the non-linear process under high optical intensity excitation via the non-equilibrium spin dynamics (carriers or magnetic atoms) in bare TIs, magnetic TIs and FM/TI bilayers. More in details, our objective is to investigate the spin-polarization dynamics, the carrier relaxation processes involving bulk and SS, including electron-magnetic impurities coupling as well as the spin texture. We will investigate the **non-linear dynamics**, with a focus on the SCC probed using THz emission spectroscopy (*UMφ - LPENS – INSP Paris*) in the ultrafast timescale (*30 fs laser pulsed excitation) with the possibility to vary the photon energy (excitation wavelength from 630 nm to 2um*) **[6].**

Nevertheless, a large effort in the modelling, electronic band structure calculations and linear response theory is now required to go ahead. In order to access the fundamental properties of the electronic band structure of FM/TI and MTI, three different methods may be proposed 1) the use and development of ***k. p*** effective Hamiltonian modelling 2) a more accurate ***sp^3*** and ***sp^3d*** (in FM/TI bilayers) slab tight-binding (***TB***) approach describing multilayers like shown recently and 3) Density functional theory (***DFT***). The effective *k. p* Hamiltonian model with reduced dimension represents an efficient way to describe the properties of the SS of TI and the possibility to study the interactions with the light in photogalvanic and photovoltaic [9] experiments. However hardly can accurately predict the SCC in the linear response theory as the TB method may do.

Post-Doc Profile (30 months)

The Post-Doc will have to develop calculations:

- to describe TI and FM/TI (*e.g.* BiSb and Co/BiSb) electronic properties and computing the Z_2-Index (possibly by TB)
- to describe FM/TI (*e.g.* Co/BiSb) REE/IREE in the linear response regime (Kubo's formula) by possibly using TB methods
- to describe TI and FM/TI (*e.g*. BiSb and Co/BiSb) photogalvanic properties by REE/IREE in the second order response regime (possibly TB)
- will investigate the SS properties in FM/TI (Co/BiSb) and MTI's as Cr and Mn-doped doped Bi_2Se_3 Bi_2Te_3 and $Bi_2Se_{3-x}Te_x$ (possibly TB or DFT).

Because the crystal structure of these bare materials possesses inversion symmetry, such computation can be performed using the Fu-Kane method. For the computation of the bulk band structure, the Slater- Koster tight-binding method may be used following Pertsova and Canali **[6]** for the tight-binding Hamiltonian, Zhang et al. **[5]** for the crystal structure and **[7]** for the tight-binding parameters. The output electronic band structure generated from the Tight-binding treatment will be used to calculate the spin-charge conversion (SCC) of the different Bi-based magnetic topological insulators materials (e.g. Cr doped) in order to discriminate the bulk and their enhanced topological

surface states contribution to the SCC and to the THz spectroscopic studies. The photogalvanic effects will be calculated in the same way at second order of the perturbation theory **[9].**

References:

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[4] Y. Xia et al., Nat. Phys. 5, 398 (2009), https://doi.org/10.1038/nphys1274

[5] H. Zhang et al., Nat. Phys. 5 438 (2009), https://doi.org/10.1038/nphys1270

[6] T.-H. Dang et al., *Applied Physics Reviews* 7, 041409 (2020) https://doi.org/10.1063/5.0022369

[7] A. Pertsova et al, New J. of Phys. 16, 063022 (2014), https://iopscience.iop.org/article/10.1088/1367-2630/16/6/063022

[8] K. Kobayashi et al., Phys. Rev. B 84, 205424 (2011), https://doi.org/10.1103/PhysRevB.84.205424

[9] L. Gao et al. Phys Rev. Research 3, L042032 (2021), https://10.1103/PhysRevResearch.3.L042032

Post-Doc skills:

- Tight-binding (sp^3 and sp^3d basis)
- Density functional Theory
- Effective Hamiltonian
- Linear response theory

Period: Position available from Oct. 2023 (30 months)

Salary: about 2890 €/month

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