Topological Spin Transport in

Quantum Materials & Entanglement Dynamics

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Abstract: In this talk, I will present theoretical spin transport features in Quantum Materials such as $MoTe_2$ and WTe_2-based materials which have recently been the subject of great attention within the broad context of Topological Quantum Matter [1]. By focusing on the monolayer limit, using DFT-derived tight-binding models and using both efficient bulk and multi-terminal formalisms and techniques [2,3], I will first discuss the emergence of new forms of intrinsic spin Hall effect (SHE) that produce large and robust in-plane spin polarizations. Quantum transport calculations on realistic device geometries with disorder demonstrate large charge-to-spin interconversion efficiency with gate tunable spin Hall angle as large as $\theta_{xy}\approx 80\%$, and SHE figure of merit $\lambda_s.\theta_{xy}\sim$ 8-10 nm, largely superior to any known SHE material [4]. Besides, I will present our theoretical prediction of an unconventional canted quantum spin Hall phase in the monolayer Td-WTe_2, which exhibits hitherto unknown features in other topological materials [5]. The low-symmetry of the structure induces a canted spin texture in the yz plane, dictating the spin polarization of topologically protected boundary states. Additionally, the spin Hall conductivity gets quantized ($2e^2/h$) with a spin quantization axis parallel to the canting direction. Our theoretical predictions for the canted QSHE findings have just been confirmed experimentally [6], and we have also shown that a perpendicular electric field could tailor the canting angle, with a 90° coherent rotation [7]. I will finally discuss the role of entanglement between intraparticle degrees of freedom in spin transport and dynamical patterns of entanglement, as enabling novel platform for generating and manipulating quantum entanglement between internal and interparticle degrees of freedom [8].

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Bio: ICREA Prof. Stephan Roche is working at the Catalan Institute of Nanosciences and Nanotechnology-ICN2 and BIST. He leads the "Theoretical and Computational Nanoscience" group which focuses on physics of Dirac materials (graphene & topological insulators) and 2D materials-based van der Waals heterostructures. He pioneered the development of linear scaling quantum transport approaches enabling simulations of billion atoms-scale disordered models (wwwlsquant.org). He studied Theoretical Physics at ENS and got PhD (1996) at Grenoble University (France); worked in Japan, Spain & Germany; was appointed as assistant Prof. in 2000, CEA Researcher in 2004 and joined ICREA in 2009. He received the Friedrich Wilhelm Bessel prize from the Alexander von Humboldt Foundation (Germany). Since 2013, he has been very active in the Graphene Flagship, currently as leader of the workpackage SPINTRONICS and is acting as DIVISION leader. Finally, he is leader and coordinator of the “Quantum Communications” activities at ICN2.