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Spin dynamics of graphene explained through supercomputing

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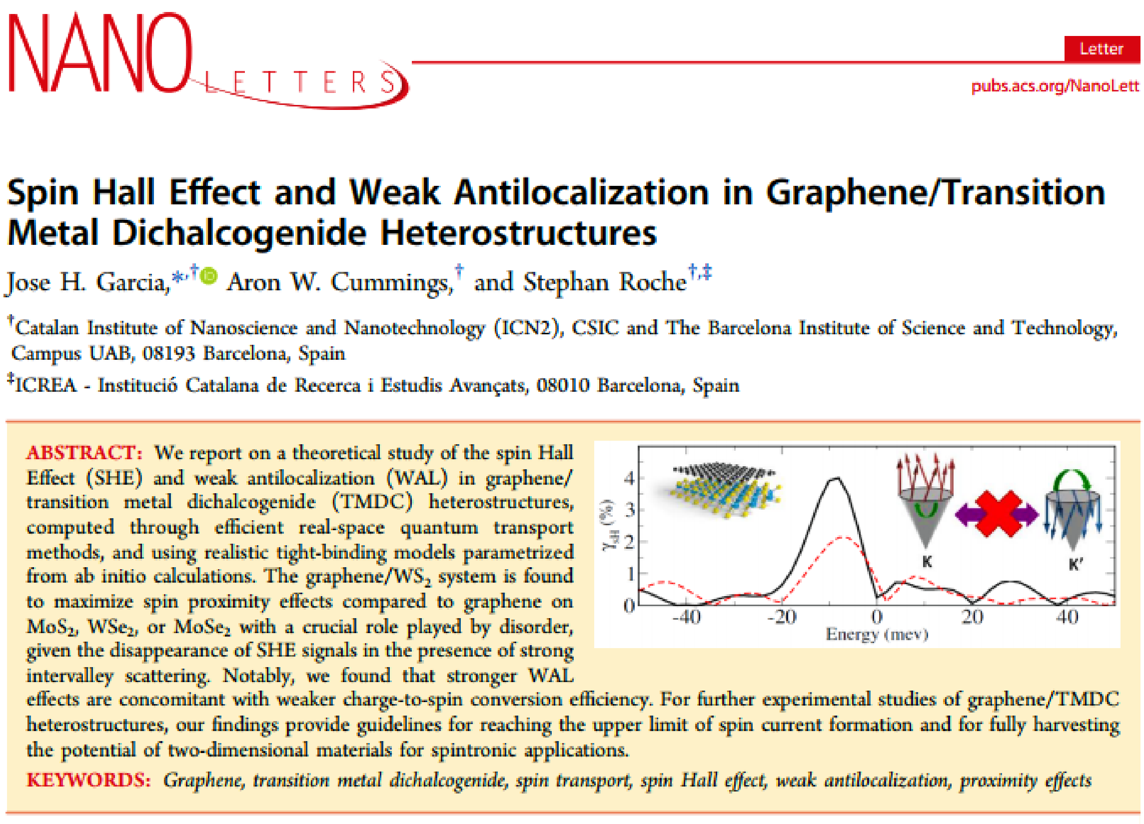

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Spin Hall Effect and Weak Antilocalization in Graphene/Transition Metal Dichalcogenide Heterostructures

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ABSTRACT: We report on a theoretical study of the spin Hall Effect (SHE) and weak antilocalization (WAL) in graphene/transition metal dichalcogenide (TMDC) heterostructures, computed through efficient real-space quantum transport methods, and using realistic tight-binding models parametrized from ab initio calculations. The graphene/WS_2 system is found to maximize spin proximity effects compared to graphene on MoS_2, WSe_2, or $MoSe_2$ with a crucial role played by disorder, given the disappearance of SHE signals in the presence of strong intervalley scattering. Notably, we found that stronger WAL effects are concomitant with weaker charge-to-spin conversion efficiency. For further experimental studies of graphene/TMDC heterostructures, our findings provide guidelines for reaching the upper limit of spin current formation and for fully harvesting the potential of two-dimensional materials for spintronic applications.

KEYWORDS: *Graphene, transition metal dichalcogenide, spin transport, spin Hall effect, weak antilocalization, proximity effects*

Credit: ICN2

In a previous study, researchers found evidence to suggest that spin-orbit coupling (SOC) was greater in graphene/transition metal dichalcogenide heterostructures than in regular graphene. In principle, this phenomenon is a necessary prerequisite for the spin Hall effect (SHE), yet subsequent tests to measure the system's SHE gave inconclusive results. In a paper published this July in *NanoLetters*, researchers of the ICN2 Theoretical and Computational Nanoscience Group, led by ICREA Prof. Stephan Roche, were able to confirm the observations of an enhanced SOC, as well as propose a reasonable explanation as to why the SHE could not be measured experimentally.

Spintronics is a branch of electronics that uses the spin of subatomic particles like electrons to store and transport information, and not just the charge as with conventional electronics. The result is devices that are faster, operate at a fraction of the energy cost and have vastly larger memory capacities. The spin Hall effect is what allows us to create and manipulate the spin, and generate a spin current. But in the previous experiment, although the SHE was taking place, the resulting spin current could barely be detected.

What ICN2 researchers did, thanks to access to the Barcelona Supercomputing Center's MareNostrum via an EU PRACE project, was to scale-up the experiment, conducting detailed and realistic simulations at the micrometer scale. As first author of the paper Dr. Jose H. García Aguilar explains, by doing so they were able to show that the conditions that enabled observation of enhanced SOC were not the same as those required to observe the SHE. Specifically, to observe the former, you need the material to be structurally defective, which creates disorder and high inter-valley scattering as the charge passes through the material. However, this high level of disorder, which emerged as significant only once the experiment had been simulated on a larger scale, was suppressing the spin current generated through the SHE, leading to the inconclusive results reported.

This study offers new insights into the spin dynamics unique to graphene, and allows us to propose new paths to achieving SHE-induced spin current experimentally in graphene-based heterostructures.

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