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Computational spin caloritronics

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Recent experimental and theoretical studies focused on spin-mediated heat currents in at interfaces between metals and insulators, where the latter can be either the barrier in a magnetic tunnel junction or a ferromagnetic insulator. A crucial parameter is the efficiency of spin injection and spin-transfer torque. In this talk, we will report realistic electronic structure calculations for two material systems. 1) The pertinent material parameter governing spin transfer and spin Seebeck effect is the spin mixing conductance that we calculate for the Silver-YIG (Yttrium-Iron-Garnett) interface. This turns out to be much larger than expected from the Stoner model. We find mixing conductance comparable to intermetallic interfaces, a surprising result that can be rationalized in terms of magnetic local moments at the interface. These results imply that the spin-mediated energy and information transmissivity of magnetic insulators is potentially much better than has been measured in early experiment, a result that has been experimentally corroborated very recently by several groups. 2). We demonstrate that the thermal spin-transfer torque (TST) in a junction Fe-MgO-Fe tunnel junctions with ultra thin barriers can amount to $10^{-7}\text{J/m}^2/\text{K}$ at room temperature, which is estimated to cause magnetization reversal for temperature differences over the barrier of the order of 10 K. The large TST for ultrathin barriers can be explained by multiple scattering due to interface states. Direct evidence for the existence of these states can be obtained by comparing shot noise calculations with recent experiments for high-quality junctions [Arakawa et al., Appl. Phys. Lett. 98, 202103(2011)]. *This work was carried out in collaboration with Xingtao Jia, Kai Liu and Gerrit E.W. Bauer.