A first-principles approach to orbital accumulation and orbital transport

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Recent first-principles calculations have predicted that, apart from the electrically induced spin currents and spin polarization, there are in fact much larger orbital angular momentum currents and induced orbital polarizations. A huge orbital Hall effect (OHE) was predicted to exist in 3d metals [1] and a huge orbital Rashba-Edelstein effect (OREE) was predicted for the symmetry-broken antiferromagnets CuMnAs and Mn_2Au [2]. Both effects do not require spin-orbit interaction (SOI) and large effects can be obtained for materials containing light atoms. This provides a perspective for future utilization of orbital angular momentum, instead of spin, as information carrier in the emerging field *orbitronics*.

I will discuss our recent linear-response theory calculations for the electrically induced out-of-equilibrium spin and orbital currents in bulk 3d ferromagnets as well as in Pt/3d-metal bilayer films [3,4]. For bulk 3d ferromagnets as Fe, Co and Ni, we show that there exists a conventional spin Hall effect (SHE), and an OHE, as well as a magnetic spin Hall effect (MSHE) and a magnetic orbital Hall effect (MOHE) [3]. The former two effects are time-reversal even, whereas the MSHE and MOHE are time-reversal odd and exist in ferromagnetic materials. These induce a transverse spin or orbital current with spin/orbital polarization along the applied electric field. The MSHE is strongly electron lifetime dependent, but in general, it is of the same size of the SHE and cannot be neglected. The OHE is the largest quantity as it doesn't require SOI, but the SHE, MSHE, and MOHE all require SOI to be non-zero.

For the Pt/3d-metal (Co, Ni, Cu) bilayer systems we compute the spin and orbital conductivities and the spin/orbital accumulation on the sides of the bilayer. The electrically induced transverse orbital current is larger than the spin current and present even without SOI. This underlines that also in the Pt/3d-metal bilayers the electrically induced orbital effects (OREE and OHE) are the primary responses, whereas the SREE and SHE are generated from these through SOI. We further compute atom-resolved response quantities that allow us to identify the contributions that lead to fieldlike or dampinglike spin-orbit torques and compare their relative magnitude, and dependence on the magnetization direction.

References:

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