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From materials to circuits: Multiscale modeling of nano-magnetic switches[1]

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Over the last decade, a rich variety of magnetic switching phenomena have appeared on the horizon, including spin torque, straintronics, Giant Spin Hall, voltage controlled magnetic anisotropy. These studies have led to the design and exploration of nanomagnetic devices such as MRAMs, STTRAMs, STNOs, CSL, ASL, stochastic, neuromorphic and so on. Each device must occupy a complex multi-dimensional phase space defined by an energy budget, a desired speed and a target read-write-retention error rate. To identify fundamental limitations and design better magnetic switches, we have developed a multiscale simulation tool that goes from material to circuit level performance metrics, and identifies key challenges along the way. At the lowest level, we start with Density Functional Theory (DFT) to identify magnetic alloys from the Heusler family that form stable half-metals. Heterojunctions and superlattices made out of these materials are predicted to give us high magnetic anisotropy and high polarization. We can then incorporate the DFT complex bands, or their simplified continuum versions, into a quantum kinetic transport solver based on the Non-Equilibrium Greens Function (NEGF) formalism to extract the tunnel magnetoresistance, spin current and spin torque. At this stage, we can add phenomenological spin-flip scattering (e.g. from magnons) as additional self-energy matrices. Finally, the current is incorporated into a micromagnetic solver that computes the results for a stochastic Landau-Lifschitz-Gilbert (LLG) equation to evaluate the switching dynamics. Instead of a Monte-Carlo sampling of the noise, we can directly evaluate the switching probability distribution using a fast Fokker-Planck approach that calibrates well with empirical models over the entire parameter range (sub-critical to super-critical switching). We discuss various ways to carry through these steps, and the challenges and opportunities we see with magnetic switching based on our simulations. [Ref: Spin Transfer Torque: A Multiscale Picture, Yunkun Xie, Ivan Rungger, Kamaram Munira, Maria Stamenova, Stefano Sanvito and Avik W. Ghosh, Nanomagnetic and Spintronic Devices for Energy-Efficient Memory and Computing, (eds J. Atulasimha and S. Bandyopadhyay), John Wiley Sons, Ltd, Chichester, UK (2016).]

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