Spin-transfer torque at finite bias from density functional theory and non-equilibrium Green's functions

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The spin-transfer torque (STT) exerted on a magnetic layer by a spin-polarized current represents a powerful handle to manipulate the magnetization. This can make magnetic random-access memories a reality. We have now implemented STTs in the electron transport code Smeagol (www.smeagol.tcd.ie), which combines density functional theory with the non-equilibrium transport formalism. In particular, we are able to compute the STT both in the linear response limit and at finite bias, and for magnets with an arbitrary complex electronic structure, including spin-orbit interaction. Examples will be provided for both magnetic tunnel junctions and spin-polarized scanning tunnel microscopy of magnetic ions on non-magnetic surfaces.