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Ab initio modeling of molecular spintronics DEREK WALDRON, VLADIMIR TIMOCHEVSKI, Dept. of Physics, McGill University, BRIAN LARADE, QuantuModeling Inc., HONG GUO, Department of Physics, McGill University — We report on theoretical studies of spin polarized quantum transport through molecular scale magnetic tunnel junctions. Our theoretical formalism is based on carrying out density functional theory (DFT) analysis within the Keldysh nonequilibrium Green's function (NEGF) formalism. The NEGF-DFT technique allows one to calculate nonlinear quantum transport features from atomic point of view. We will report these features for systems such as Ni-bezenedithiol(BDT)-Ni molecular magnetic tunnel junction, conventional Fe-MgO-Fe device, and spin injection through Fe-GaAs interfaces, including all the microscopic material properties.

Hong Guo
Dept. of Physics, McGill University

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