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Nonlinear and Nonequilibrium Spin Injection in Magnetic Tunneling Junctions

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Quantitative analysis of charge and spin quantum transport in spintronic devices requires an atomistic first principles approach that can handle nonlinear and nonequilibrium transport conditions. We have developed an approach for this purpose based on real space density functional theory (DFT) carried out within the Keldysh nonequilibrium Green's function formalism (NEGF). We report theoretical analysis of nonlinear and nonequilibrium spin injection and quantum transport in Fe/MgO/Fe trilayer structures as a function of external bias voltage. Devices with well relaxed atomic structures and with FeO oxidization layers are investigated as a function of external bias voltage. We also report calculations of nonequilibrium spin injection into molecular layers and graphene. Comparisons to experimental data will be presented. Work in collaborations with: Derek Waldron, Vladimir Timochevski (McGill University); Ke Xia (Institute of Physics, Chinese Academy of Science, Beijing, China); Eric Zhu, Jian Wang (University of Hong Kong); Paul Haney, and Allan MacDonald (University of Texas at Austin).