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Towards ab-initio calculations for antiferromagnetic metal spintronic devices. PAUL HANEY, DEREK WALDRON, ALVARO NUNEZ, REM-BERT DUINE, HONG GUO, DEREK WALDRON — In conventional spintronics, the electron's spin degree of freedom is exploited to construct systems which exhibit behavior of practical importance and fundamental scientific interest. The prototypical system is a heterostructure which consists of alternating layers of ferromagnetic and paramagnetic materials. Such a system is used to study GMR and spin transfer torque, the two most important phenomena in spintronics today. In GMR, the relative orientation of magnetic layers affects the current flowing through a heterostructure, while in spin transfer the current flowing through the structure effects the orientation of the magnetic layers. It is of interest to consider what type of effects occur in structures containing antiferromagnetic materials. To this end, realistic calculations of GMR and spin transfer in antiferromagnetic heterostructures are presented. The calculations are carried out using ab-initio NEGF methods, using the LSDA extended to noncollinear magnetic configurations. Preliminary results of a Cr-Au-Cr structure are presented as an example of an experimentally realizable antiferromagnetic system.

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