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First-principles theory of current-induced spin torques in non-collinear antiferromagnets ALLAN MACDONALD, HUA CHEN, The University of Texas at Austin, YIMING WU, Peking University, YASUFUMI ARAKI, Tohoku University — We propose a new theoretical approach for calculating current induced torques in hybrid systems containing magnetic and heavy metal thin films. The theory is based on ab-initio density functional theory (DFT) and appeals explicitly to the local-spin-density approximation for exchange and correlation. Because the effective magnetic field from exchange and correlation is everywhere parallel to the spin-density in the ferromagnet, it does not contribute to the current-induced torque, which is due entirely to spin-orbit coupling near heterojunctions involving heavy metals. The theoretical picture can be combined with any theory of the electronic steady state produced by electrochemical potential gradients, and involves response of the single-particle density matrix that is partially diagonal and partially off-diagonal in an unperturbed eigenstate representation. The theory is formulated using the basis of Wannier functions and can be readily interfacing with existing DFT codes. This approach predicts strong current-induced torques due to either antiferromagnetic or non-magnetic heavy metal layers. As an illustration, we use it to calculate specifically the spin torque in a ferromagnet induced by an adjacent noncollinear antiferromagnet (Mn3Ir).

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