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Optimizing Co concentration in Co_xFe_{1-x}/MgO/Co_xFe_{1-x} magnetic tunnel junctions to maximize tunneling magnetoresistance[1]
JONATHAN TRINASTIC, YAN WANG, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida, Gainesville, FL 32611
— $Fe_{1-x}Co_x$ /MgO magnetic tunnel junctions (MTJs) are of great experimental interest due to large differences in conductance between parallel and anti-parallel spin alignment in the electrodes that lead to high tunneling magnetoresistance (TMR). However, the optimal Co concentration in the electrodes that maximizes TMR is still under investigation (Bonell et al 2012,*PRL,*108,176602). Using first-principles calculations, we compare the conductance and TMR of $Fe_{1-x}Co_x$/MgO junctions using 1) disordered electrodes modeled with the virtual crystal approximation (VCA), and 2) ordered $Fe_{0.75}Co_{0.25}$ and $Fe_{0.50}Co_{0.50}$ electrodes. For disordered electrodes, we find that the optimal Co concentration varies between 20 and 30 percent and TMR decreases with MgO barrier thickness. For ordered electrodes, pure Co electrodes exhibit the highest TMR for a thin MgO barrier; however, $Fe_{0.75}Co_{0.25}$ electrodes demonstrate the highest TMR for a thicker MgO barrier, replicating recent experimental results. In all cases, a decrease in anti-parallel transmission drives the TMR increase.

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Jonathan Trinastic
Department of Physics and Quantum Theory Project,
University of Florida, Gainesville, FL 32611

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