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First principles Modeling of Magnetoresistance in Magnetic Memory devices KURT STOKBRO, MORTEN STILLING, Atomistix Inc, KARSTEN FLENSBERG, Copenhagen University — We have performed first principles calculations of the zero- bias conductance and TMR for crystalline Fe-MgO-Fe MTJs, and studied the effects of different oxide layers in the Fe/MgO interface, and the effects of structural "disorder" in the device. We find that such "defects" in the atomic structure have strong effects on the conductance. We use the result of the calculations to rationalize recent experimental findings. The simulations have been done with the software package Atomistix ToolKit (ATK), which is based on density functional theory (DFT) and non-equilibrium Green's functions (NEGFs).

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