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Atomic and electronic properties of $Ni/Al_2O_3/Ni$ magnetic tunnel junction YOU LIN, University of South Florida, IVAN OLEYNIK, University of South Florida — Numerous experimental and theoretical investigations show that the spin-polarization of the tunneling current in magnetic tunnel junctions (MTJs) is not an intrinsic property of the ferromagnet alone, but depends on the electronic properties of the insulator and the ferromagnet-insulator interface. We report the results of first-principles density-functional studies of $Ni\_/Al_2\_O_3\_/Ni$ MTJs. The atomic structure has been studied for different interface terminations. The interfacial energetics was quantified based on the work of separation and the most stable interfacial structures have been identified. The electronic and magnetic properties have been thoroughly analyzed in the framework of local densities of states. The possibility of strongly-correlated electronic effects has also been considered by performing additional LDA+U calculations of interfacial electronic structure. We will discuss various factors that might contribute to spin polarization of the tunneling current in the MTJs.

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