Abstract Submitted
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**Extended Hückel theory based transport model for Fe-MgO-Fe magnetic tunnel junctions**[1] TEHSEEN RAZA, ECE Purdue University, JORGE CERDA, ICMM-CSIC, Cantoblanco, Madrid, Spain, HASASN RAZA, ECE University of Iowa — Fe-MgO-Fe magnetic tunnel junction devices have attracted increased attention due to their preferential symmetry filtering of the half-metallic $\Delta_1$ band in Fe, which results in a high tunnel magnetoresistance ratio. Motivated by their applications in memory and sensor devices, we present an extended Hückel theory (EHT) model coupled with the non-equilibrium Green's function formalism [1] to efficiently calculate the transport through these devices. We propose EHT parameters for MgO benchmarked with the k-resolved projected density of states calculated using the local density approximation of the density functional theory. We further optimize the MgO parameters to have the experimental band gap. These parameters are transferrable to various MgO thicknesses and the transport results match well with earlier calculations. [1] T. Z. Raza J. I. Cerda and H. Raza, in preparation. We are thankful to R. Hoffmann, R. Berger and S. Datta for useful discussions and NCN for computational resources.

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