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Real space first-principles derived semiempirical pseudopotentials applied to tunneling magnetoresistance[1] KIRK BEVAN, Oak Ridge National Laboratory, Materials Science and Technology Division, TONY LOW, Purdue University, Department of Electrical and Computer Engineering, HONG GUO, McGill University, Centre for the Physics of Materials and Department of Physics
— We present a real space density functional theory (DFT) localized basis set semiempirical pseudopotential (SEP) approach. The method is applied to iron and magnesium oxide, where bulk SEP and local spin density approximation (LSDA) band structure calculations are shown to agree within approximately 0.1 eV. Subsequently we investigate the qualitative transferability of bulk derived SEPs to Fe/MgO/Fe tunnel junctions. We find that the SEP method is particularly well suited to address the tight binding transferability problem because the transferability error at the interface can be characterized not only in orbital space (via the interface local density of states) but also in real space (via the system potential). To achieve a quantitative parameterization, we introduce the notion of ghost semi-empirical pseudopotentials extracted from the first-principles calculated Fe/MgO bonding interface. In general the results underscore the need for separate tight binding interface and bulk parameter sets when modeling conduction through thin heterojunctions on the nanoscale.

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