Ab initio magnetocrystalline energy calculations of zinc blende multilayer with ferromagnetic dopants

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We investigate the magnetocrystalline anisotropy energy (MAE) of zinc blende ferromagnetic multilayer [1] using the local spin density approximation based on the density functional theory (DFT) and Hubbard model (LSDA+U). We take into account the effect of strong electronic correlations and spin-orbit coupling in the full potential linear muffin tin orbital (FP-LMTO) calculations [2].

The MAE distributions for different number of atomic multilayer differences between the majority and minority spin orbital moments for the magnetization parallel and perpendicular to the c-axis, have been obtained. Calculated MAE's and density of states (DOS) functions have been analyzed. Calculation results show that MAE mainly due from changes in occupation number of ferromagnetic dopants minority spin levels for different magnetization directions.

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