

The objective of this work is to employ spin-polarized density functional theory (SDFT) calculations for the exploration of ultrathin magnetic films with large magnetic moments and a strong perpendicular anisotropy. Ultrathin monolayer films of $\text{Fe}_{1-x}\text{Co}_x$ (with $x = 0, 0.25, 0.5, 0.75$ and 1) on $\text{Rh}(001)$ were addressed to study their magnetic properties using the all-electron full-potential linearized augmented plane wave (FLAPW) method in film geometry. We studied the magnetic order of these films including relaxations of the topmost layers. $\text{Fe}_{1-x}\text{Co}_x$ monolayer films were found to be ferromagnetic (FM) in a broad range of Co content x with a maximum magnetic moment of $2.8 \mu_B$ and of an out-of-plane magnetocrystalline anisotropy of 0.25 meV per magnetic atom at $x = 0.5$. The SDFT results were mapped onto a classical Heisenberg model, demonstrating FM Fe-Co and Co-Co coupling, while the Fe-Fe interaction is antiferromagnetic (AFM) on $\text{Rh}(001)$. The ordering temperature was estimated to be well above room temperature (482 K). Using SDFT calculations, we have studied the magnetic states including collinear and noncollinear magnetic coupling in $\text{Fe}_{1-x}\text{Co}_x$ ultrathin films on $\text{Rh}(001)$ substrate. We found for 7 layers of Rh spacer an interlayer exchange coupling (IEC) with absolute values of 3.4 and 2.9 meV per 3d atom corresponding to the two magnetic films Co/Rh/Co and FeCo/Rh/Co , respectively. These films show a very large IEC compared to that obtained for Fe/Ag/Fe or Fe/Au/Fe films, which is IEC is one order of magnitude smaller. We found also that the IEC oscillates with increasing Rh spacer thickness, i.e. the Rh spacers mediate an interlayer coupling which couples the magnetizations either ferromagnetically or antiferromagnetically depending on the spacer thickness. Our calculations give an antiferromagnetic (AFM) coupling for 5 layers of Rh spacer and a ferromagnetic (FM) one for 7 layers, as has been experimentally detected for thicker magnetic films. The exchange coupling energy including spin orbit coupling was calculated for the $n\text{FeCo}/5\text{Rh}/\text{Co}$ films in the framework of the constrained SDFT. A strong perpendicular anisotropy of 0.15 meV per 3d atom has been found for the $2\text{FeCo}/5\text{Rh}/\text{Co}$ film while the single FeCo monolayer system $\text{FeCo}/5\text{Rh}/\text{Co}$ preferred an in-plane magnetic anisotropy. This result suggests that the competition between IEC and magnetic anisotropy of coupled films may result in noncollinear ordering. The results of the constrained SDFT are mapped onto the bilinear-biquadratic exchange coupling model of the Hamiltonian including the uniaxial anisotropy term. We found a values of 3.55 and 0.62 meV per 3d atom for the bilinear and biquadratic coupling constants respectively