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Photo-Switching of Magnetization in Iron Nanoparticles NABIL AL-AQTASH, ALEXANDER HOSTETTER, RENAT SABIRIANOV, University of Nebraska at Omaha — We report the theoretical studies of light induced switching in core-shell nanoparticles. The core of the nanoparticle is made of Fe coated with the shell of azobenzene. The latter is a photochromic material with the reversible *trans-cis* photoisomerization upon irradiation by UV and visible light. The magnetization of nanoparticles can be reversibly switched by using specific wavelengths of light. *trans-cis* photoisomerization of azobenzene induces both the change in surface local magnetic moments and alters the exchange interactions on the surfaces of the nanoparticles. These two mechanisms can lead to induced magnetization switchable by light pulse. We study the effects of photoisomerization of azobenzene on iron (Fe) nanoparticle. Ab initio calculations using SIESTA code show that the ferromagnetic (FM) and antiferromagnetic (AFM) exchange interaction in Fe dimer increase by 40% due to photoisomerization of azobenzene. While an infinite flat Fe monolayer shows variation on the exchange interactions on the surfaces as result of photoisomerization. The local magnetic moments of Fe sheet increase by 6% due to photoisomerization. Using an *ab initio* parameterization of magnetic interactions, we propose statistical model based on competing exchange interactions for the investigation of Fe nanoparticle magnetization. We performed Monte Carlo simulations of magnetization of the core-shell nanoparticle as a function of temperature. The results show that Fe nanoparticles magnetization at room temperature can change by at least 40% due to photoisomerization of azobenzene.

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