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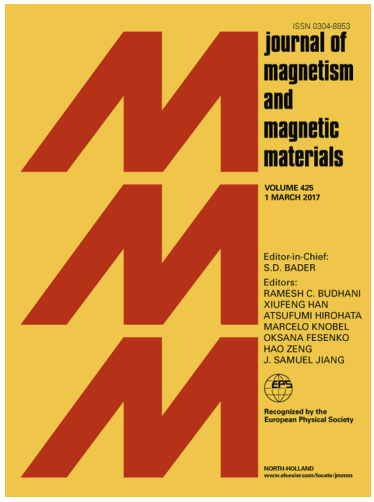

Spin ordering in oxide nanoclusters without magnetic element atoms

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ACCEPTED MANUSCRIPT

Spin ordering in oxide nanoclusters without magnetic element atoms

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Abstract

The calculations of spin effects in 20 Si_nO_{2n+m} nanoclusters with $10 \geq m \geq 5$ and $m \geq 1$ are presented. They include search for the equilibrium atomic structure, the calculations of electron spectra and the energy of different spin orderings. It was found that all Si_nO_{2n+m} clusters have spin moments, which are located on radical O atoms at the cluster surface. Long radical-to-radical distance weakens their exchange interaction, so energy differences between ferro-, ferri-, and antiferromagnetic states are of 0.01 eV or lower, gaining 0.046 eV only in Si_6O_{13}. We analyze this magnetism in terms of electron spectra and individual radical groups. Its similarity to popular molecular magnets based on organic radicals is noticeable. The stability of these Si_nO_{2n+m} clusters in O_2 atmosphere, as well as their relation to silicon technology, is of particular interest for spintronics.

Keywords: oxide nanoclusters, metal phthalocyanines, spintronics, Stoner criterion

1. Introduction

The creation of materials combining semiconducting and magnetic properties remained a challenging problem of spintronics for over last two decades. For many years diluted magnetic semiconductors were thought as most promising materials for this problem. However low stability against magnetic atoms segregation, which was found in these materials, cast doubt on their potential harnessing [1]. The fast development of nanotechnology, as well as the unique properties of nanoparticles gave a new impetus to tackle this problem by searching for adequate nanomaterials. A potential application area of such nanoparticles is very wide: future information technology, quantum computations, spintronic devices, bimodal sensors, etc. One way to construct them is the doping of nonmetallic nanoparticles by Mn and other magnetic 3d-elements [2]. It replicates the engineering of bulk diluted magnetic semiconductors and can share some of its problems. Another way is addressed to inherent spin polarization of nanoparticles, which can exist at their surface. One such example, which may be pointed out, is the experimental detection of spins at the surface of CdSe nanocrystals passivated by TOPO (tri-n-octylphosphine oxide) [3]. As was argued later [4], the reordering of spins activates the radiative recombination of dark excitons in CdSe nanocrystals, so photoluminescence is controlled by spin flip-flop processes at the nanocrystal surface. The other example of surface spin polarization refers to oxide nanoparticles. The first-principles calculations [5, 6] revealed that in oxygen atmosphere the equilibrium Mg_nO_m and Si_nO_m nanoclusters have excessive O atoms, comparing to the stoichiometric MgO and SiO_2 compositions. These are precisely those O atoms, which are responsible for spins at the cluster surface. Probably, this surface spin polarization has much in common with molecular magnets based on organic radicals, which are intensively studied beginning from 1990's [7]. Similar phenomenon should exist in many oxide nanomaterials and possess special features that motivates its in-depth study.

In this investigation we calculate the spin properties of 20 Si_nO_{2n+m} nanoclusters with $10 \geq n \geq 5$ and $m \geq 1$ ($\sim$ 1 nm of size), considering them as

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