Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

d0 ferromagnetism in nanocrystals[1] YURI DAHNOVSKY, VITALY PROSHCHENKO, Univ of Wyoming — We study d^0 ferromagnetism in ZnS and ZnO quantum dots (QDs) and nanowires (NW). To find the magnetization of the medium and large size nanocrystals (NC) we introduce the surface-bulk (SB) model where the separately calculated surface and bulk contributions to the total magnetic moment allows us to find the magnetization for a large nanocrystal (NC). For nanowire calculations the accuracy of the SB model varies from 0.2% to 21% depending on the Zn vacancy concentrations on the NC surface and in the NC core. We find that the higher the concentration of the Zn vacancies, the larger the total magnetic moment in the nanocrystal, however the magnetic moment increase faster for quantum gots rather than for nanowires. We also study the cases where the concentrations of Zn vacancies can be different on the NC surface and in the core. From the comparison of the experimental and theoretical NW magnetic moments we find that the experimental magnetization is $1.4 \cdot 10^3$ smaller than the calculated one. Such a huge discrepancy can be explained from the assumption that not all magnetic moments due to Zn vacancy participate in the ferromagnetism and there are some regions with zero magnetism and uncoupled (paramagnetic) spins.

[1]DOE, No. DEFG02-10ER46728

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Date submitted: 03 Nov 2016 Electronic form version 1.4