

Abstract Submitted  
for the MAR09 Meeting of  
The American Physical Society

**Site occupancy and magnetic properties of aluminum substituted barium hexaferrite** AMITAVA MOITRA, SUNGHO KIM, SEONG-GON KIM, Mississippi State University, YANG-KI HONG, University of Alabama, STEVEN C. ERWIN, Naval Research Laboratory — Aluminum substituted barium hexaferrite has been studied using density functional theory (DFT). The substitution has been carried out for  $\text{BaFe}_{12-x}\text{Al}_x\text{O}_{19}$  from  $x = 1$  to  $x = 3$  in steps of 0.5. With the aid of accurate DFT study, our result show that the  $\text{Al}^{3+}$  ions preferentially occupy the 2a and 12k site, unlike the previously reported 4f2, 2a, 4f1, and 12k sites. Our result confirms the experimental fact that with increasing of Al substitution the total magnetic moment monotonically decreases. We also present a possible reason of the site preference of 2a and 12k.

Seong-Gon Kim  
Mississippi State University

Date submitted: 20 Nov 2008

Electronic form version 1.4