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Site occupancy and magnetic properties of aluminum substituted barium hexaferrite AMITAVA MOITRA, SUNGHO KIM, SEONG-GON KIM, Mississippi State University, YANGKI HONG, University of Alabama, STEVEN ERWIN, Naval Research Laboratory — Aluminum substituted barium hexaferrite has been studied using density functional theory (DFT). The substitution has been carried out for $BaFe_{12-x}Al_xO_{19}$ from x = 1 to x = 3 in steps of 0.5. With the aid of accurate DFT study, our result show that the 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.

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