Design of high-coercivity $Fe_{16-x}Al_xN_2$ alloy

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Iron nitrides ($Fe_{16}N_2$) have recently attracted considerable attentions for the future rare-earth (RE) free permanent magnets (PMs) due to its low cost and high magnetization compared to other RE-free magnetic materials. In spite of such excellent magnetic properties, its application has been limited by relatively low coercivity. Here, combining the first-principles density functional theory calculations and the alloy theoretic automated toolkit (ATAT), we extensively investigated the structure evolution, stability and magnetic properties of $Fe_{16-x}Al_xN_2$ alloys as a function of Al contents. We find that substituting Fe by Al in $Fe_{16}N_2$ with Co/Fe ratio=0.14 can increase the coercivity by about 300% compared to the pristine $Fe_{16}N_2$. We expect our findings provide an important insight to fabricate optimal $Fe_{16-x}Al_xN_2$ alloy with high coercivity.

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