First-principles prediction of novel $Fe_{14}M_2N_2$ (M=Al, W, Zr) alloys with high coercivity

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$Fe_{16}N_2$ has a potential applications as one of the promising rare-earth-free permanent magnets due to its extremely high magnetization. However, the low coercivity of $Fe_{16}N_2$ hinders its practical application. Here, using density functional theory calculations, we explored the change of tetragonality, volume and magnetization in various $Fe_{14}M_2N_2$ (M=Al, W, Zr) alloys depending on atomic position of two M atoms. We find that a $Fe_{14}Zr_2N_2$ alloy has a tetragonality of 1.29 and exhibit almost ten times higher coercivity than the $Fe_{16}N_2$ coercivity, which will be desirable for the application. We expect that our results provide essential information to understand the underlying mechanism related to coercivity, and develop novel $Fe_{16}N_2$–based permanent magnets with high coercivity.

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