

Supporting Information

Electronic structures and magnetic properties of rare-earth-free permanent magnet α'' -Fe₁₆N₂: first-principles calculations†

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[†] Electronic supplementary information (ESI) available.

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S1. The dynamical stability of α'' -Fe₁₆N₂

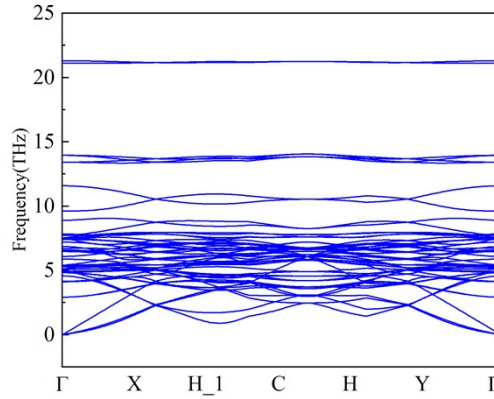


Fig. S1 Phonon dispersion curves of α'' -Fe₁₆N₂.

S2. Projected density of states of α'' -Fe₁₆N₂

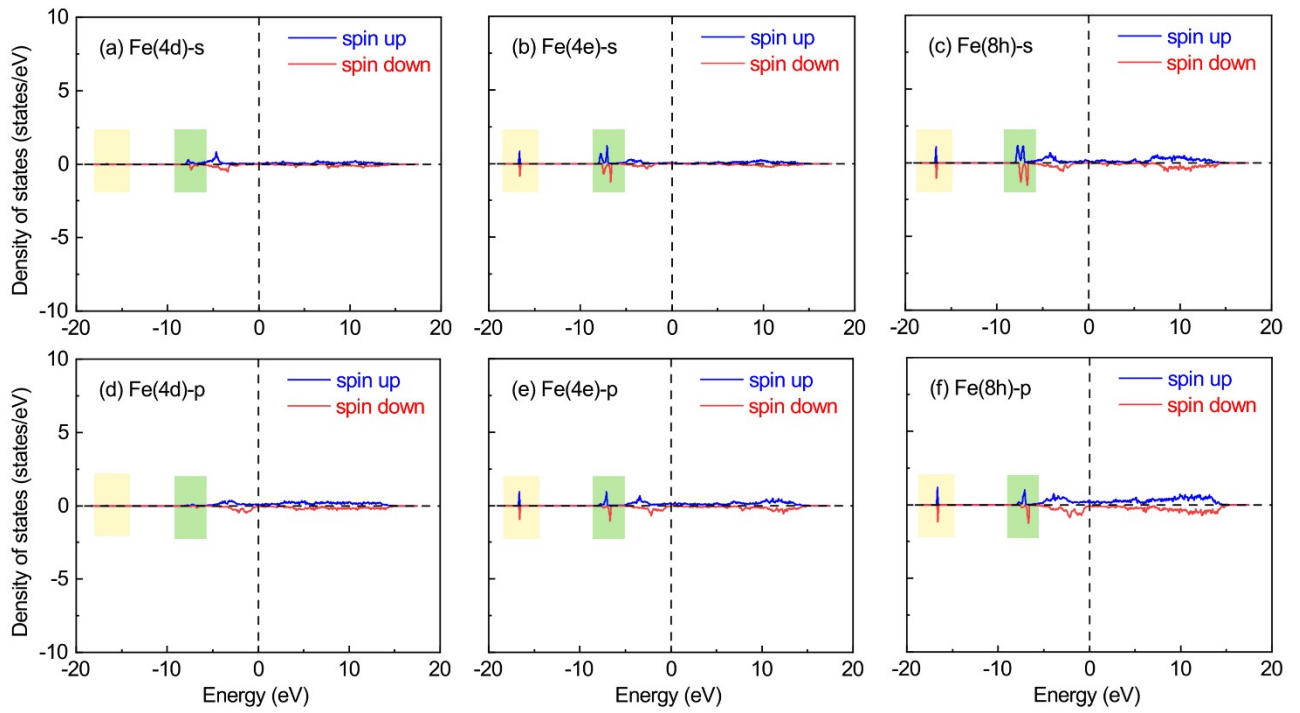


Fig. S2 Spin-polarized site-projected density of states of *s* orbit (a)Fe(4d)-*s*, (b)Fe(4e)-*s*, (c)Fe(8h)-*s*, and projected density of states of *p* orbit(d)Fe(4d)-*p*, (e)Fe(4e)-*p* and (f)Fe(8h)-*p*.

S3. The band of γ' -Fe₄N

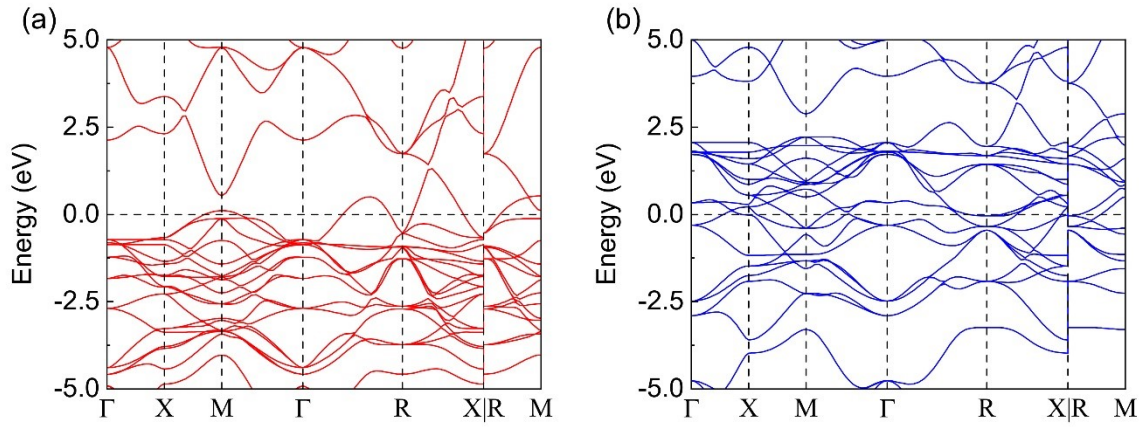


Fig. S3 The band structures of γ' -Fe₄N, (a) spin up, (b) spin down.

S4. The relationship between exchange parameters and atomic distances

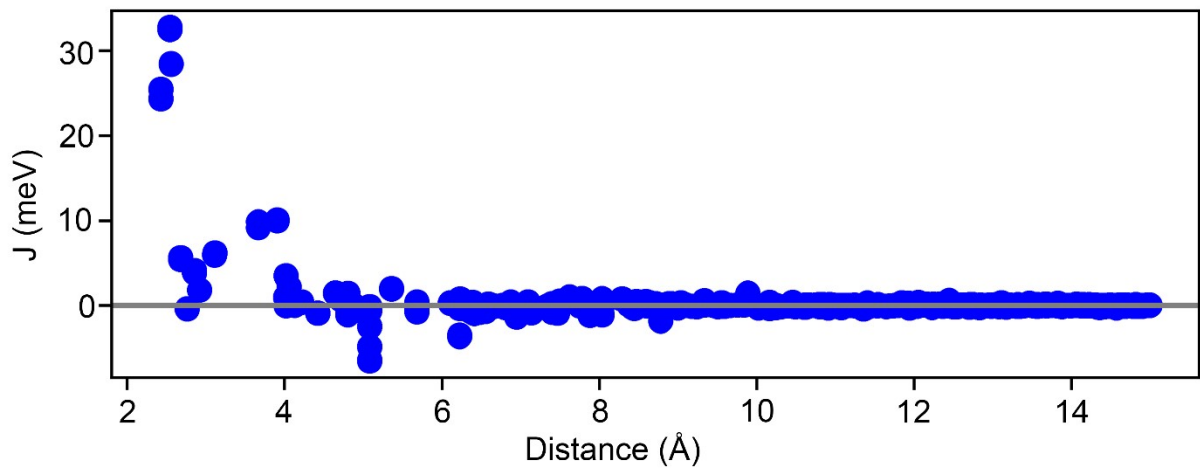


Fig. S4 The relationship between exchange parameters and atomic distances