Supporting Information

Synthesis and characterization of the strong ferromagnetic and high

hardness intermetallic compound Fe₂B

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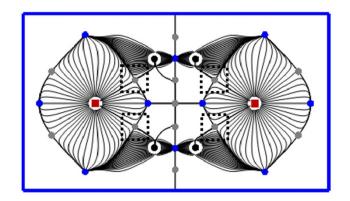


Fig S1. Gradient paths and critical points derived from AIM analysis for Fe_2B , Gray spheres represent BCPs, black spheres represent B, and red squares represent Fe. Gray spheres in dashed line boxes represent BCPs between Fe and B.

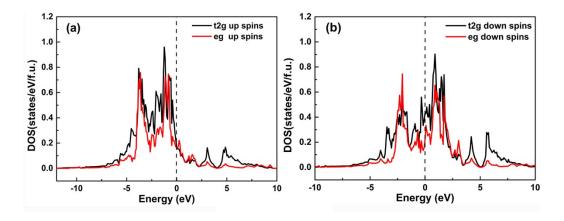


Fig S2. The calculated DOS with spin-polarization for up spins (a) and down spins (b) in e_g and t_{2g} orbitals