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Defect-Induced Magnetism in BaZnF4 QINFANG ZHANG, SEIJI YUNOKI, Computational Condensed Matter Physics Laboratory, RIKEN, Wako, Saitama 351-0198, Japan — By first-principles density functional theory with generalized gradient approximation(GGA), oxygen(nitrogen)-doped $BaZnF_4$ with O(N) substituting F at concentrations 3.125% has been demonstrated to exhibt a ferromagnetic behavior. The results show that the strong localization of defect states favors spontaneous spin polarization and local moment formation. Defect manipulation mediates long-range magnetic interaction, which opens a new route to design high-Tc diluted magnetic semiconductors(DMS).

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