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First-principles study of the magnetic and electronic properties of NiAs-type FeSe WEIDONG LUO, XIAOLE ZHANG, Shanghai Jiao Tong University, China — FeSe exhibits the NiAs-type hexagonal structure under external pressure or under certain growth conditions at ambient pressure. The superconducting transition temperature of alpha-FeSe initially increases and then decreases when external pressure is applied, in which the NiAs-type FeSe is considered as the competing phase to the superconducting alpha-FeSe. We study the magnetic and electronic properties of the NiAs-type FeSe using first-principles calculations. The ferromagnetic (FM) and several antiferromagnetic (AFM) configurations of NiAs-type FeSe have been studied, and we observe dependence of the electronic structure on its magnetic configuration of NiAs-type FeSe. The results of theoretical calculations are compared to experimental observations.

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