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Phase Transition, Magnetic and Electronic Properties of Iron Mononitride: First-Principles Calculations

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ABSTRACT: The stability, phase transition, magnetism and electronic properties of five different iron mononitride (FeN) phases are systematically studied using first-principles calculations. The results show that ZnS-FeN structure is the most stable phase at the equilibrium lattice, and the sequence of phase transition is according to ZnS→NiAs→wurtzite. Our magnetic analysis demonstrate that the ZnS, CsCl and wurtzite structures are nonmagnetic, while the NaCl and NiAs phases under high-pressure are magnetic, holding 2.27 and 1.61 μ_B per Fe atom, respectively. The magnetic moments increase with increasing of the volume for all considered structures.

Keywords: Iron mononitride; Phase transition; Electronic property; First-principles

1. Introduction

Iron nitrides (FeN) are known to be industrial and commercial compounds with versatile physical properties, such as outstanding magnetic properties [1,2]. Recent studies show that iron nitrides can be used as efficient catalysts [3,4] and a potential treatment of cancer cells [5]. Many investigations on FeN have been reported in recent years because mononitride has high N-content and is considered to be an interesting material in spintronics [6]. To date, five FeN structures, i.e., NaCl-, ZnS-, CsCl-, wurtzite- and NiAs-type have been reported. For NaCl- and ZnS-type