γ'-Fe_4N: facts, hypotheses and open questions

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By reviewing the experimental and theoretical literature on γ'-Fe_4N, and by a systematic survey of predictions by the LDA, PBE, WC, LDA+U (2×), PBE+U (2×) and B3PW91 exchange-correlation functionals, the structural, magnetic and hyperfine properties of this material as well as their pressure dependencies are interpreted. The hypothesis is put forward that γ'-Fe_4N as found in Nature is exactly at a sharp transition between low-spin and high-spin behaviour. PBE+U (U=0.4 eV) is identified as the most accurate exchange-correlation functional for this material, although it is needed to fix the magnetization at the experimental value to obtain a satisfying description. Remaining disagreement between theory and experiment is pointed out. A recent experimental claim for a giant magnetic moment in γ'-Fe_4N is discussed, and is not reproduced by our calculations.

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