

First Principles Study of α -NbSi₂N₄ Ground State Magnetic Properties

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Abstract. The magnetic ground state of intercalated monolayer α -NbSi₂N₄ is investigated using first principles calculations. Recent debate on conduction character of the ground state questions importance of a proper description of the Nb *d*-electrons. Here we discuss the effect of the Hubbard on-site potential on the magnetic splitting of the conduction band resulting in the transition from the conducting to the semiconducting state. We determine exchange parameters for nearest and second nearest neighbours, and magnetic anisotropy parameters for classical Heisenberg model on a triangular lattice of the Nb atoms. The critical temperature $T_c = 440.3$ K for ferromagnet - paramagnet transition was determined using Monte Carlo simulation.

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