

Magnetic and Electronic Properties of Monolayer α -NbSi₂N₄

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Abstract. The newly discovered family of intercalated monolayers with the structural formula MA₂Z₄ has generated significant interest due to their diverse range of physical properties. In this talk, we focus on the NbSi₂N₄ monolayer, highlighting its potential as a two-dimensional ferromagnet with promising magnetic, thermal, and optical characteristics for future spintronic applications. Using density functional theory (DFT), we investigate its mechanical stability and the possibility of charge density wave formation. The dielectric properties described by the electronic susceptibility are analyzed within the Random Phase Approximation. The particular attention was paid to the influence of overlap matrix elements in comparison with constant matrix element approximation. Optical conductivity and orbital magnetization are studied through Berry curvature calculations, employing an effective model based on a localized Wannier basis. The magnetic behavior is examined within the framework of a classical Heisenberg model with a uniaxial anisotropy term. The model parameters are extracted by mapping the total electronic energies of various magnetic configurations onto the Heisenberg spin model. Finally, we present the computed magnon dispersions and discuss the Curie temperature obtained via Monte Carlo simulations.

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