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Spin spiral state in hexagonal NiS<sup>1</sup> RAQUEL LIZARRAGA<sup>2</sup>, ERIK HOLMSTROM<sup>3</sup>, Instituto de Ciencias Fisicas y Matematicas, LARS NORDSTROM<sup>4</sup>, OLLE ERIKSSON<sup>5</sup>, Department of Physics and Astronomy, SWARUP PANDA<sup>6</sup>, INDRA DASGUPTA<sup>7</sup>, D.D. SARMA<sup>8</sup>, Indian Institute of Science — Previous nesting function calculations on NiS have found instabilities for the magnetic ordering vectors q=(2/3,2/3,0) and q=(1/2,2/9,1) suggesting that the magnetic structure of NiS is non- collinear which does not agree with the experimentally determined antiferromagnetic state. We investigated the electronic and magnetic structure of NiS by means of a full-potential linearized augmented plane wave method within the local spin density approximation plus the Hubbard parameter U. Our method is specially suitable to study noncollinear magnetism where the magne- tization density is allowed to vary in magnitude and direction continuously everywhere in space. Our results show that the ground state is metallic and that the antiferromagnetic state is almost degenerate with spin spirals along certain directions of the Brillouin zone.

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