The curious case of NiS

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NiS, exhibiting a text-book example of a first-order phase transition and accompanied by a host of unusual properties at the low temperature, has been variously described in terms of conflicting descriptions of its ground state during the past several decades. We calculate these physical properties within a first-principle approach based on the density functional theory and establish that all experimental data can be understood in terms of a rather unusual ground state of NiS that is best described as a self-doped, nearly compensated, antiferromagnetic metal, thereby providing a resolution to an age-old controversy. We trace the origin of this novel ground state to the specific details of the crystal structure, band dispersions and a sizable Coulomb interaction strength that is still sub-critical to drive the system in to an insulating state.

The results that will be discussed in this talk are based on unpublished results arising from a collaborative effort between the following people: Swarup Panda, Indra Dasgupta and D. D. Sarma.

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Relevant past literature:

Phase transition: Sparks *et al*, JAP 34,1191(1963); Trahan *et al*, PRB,2,2859(1970)

Transport: Rechard *et al*, J. App Phys,44,1682(1973)

Magnetic properties: Sparks *et al*, JAP,34,1191(1963) ; Coey *et al*, PRL,32,1257(1974)

Hall data: Ohtani *et al*, J. Phys soc Japan,37,701(1974);

Photoemission investigations: Nakamura *et al*, PRL,73,2891(1994); Sarma *et al*, PRL,80,1284(1998)

Optical data: Barker *et al*, PRB,10,987(1974); Okamura *et al*, SSC,112,91(1999)

Earlier theoretical work: Anisimov *et al*, PRB,44,943(1991); Usuda *et al*, J. Phys Soc Japan,69,744(1999)