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Pressure effects on the electronic properties of super- conducting FeS CESARE TRESCA, GIANNI PROFETA, Department of Physical and Chemical Sciences, University of L'Aquila, GIANLUCA GIOVANNETTI, MASSIMO CAPONE, International School for Advanced Studies (SISSA) , Trieste (ITALY) — We present first-principle Density- functional Theory (DFT) results on the electronic and magnetic properties of the recently discovered superconducting FeS and their variation under high pressure conditions. The DFT band structure of FeS is sensibly different with respect to the other members of the same family: a fully occupied d_{xy} band at the Γ-point is predicted. We find that the stripe-antiferromagnetic phase is the most stable magnetic solution, with different magnetic phases having comparable energies signaling a tight competition. Including local interactions treated within Dynamical Mean-Field Theory, we find significant correlation effects with orbital-dependent strength and character. High pressure conditions, experimentally found to enhance the superconducting critical temperature, produces a strong variation of the topology of the Fermi surface, disappearance of the magnetic properties and a reduction of the correlation effects. These predictions, on a new and unexplored material, add new aspects for the understanding of the iron-chalcogenides superconductors, possibly opening new research perspectives on the subject.

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