Spin Density Wave In Chromium Under High Pressure

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The phase diagram of the magnetic phases of body-center cubic chromium is elucidated from a simple Hamiltonian taken into account the essential nearest and next nearest neighbor spin-spin interactions. It is shown that the relative stability of various magnetic structures is determined by a delicate balance of these interactions. This is confirmed by First Principles density functional calculations augmented with a model Hubbard Hamiltonian. The results also show the magnetic structures of Cr are very sensitive to the lattice constant and the choice of the Hubbard U parameter. The electronic of the magnetic phases at ambient pressure can be described adequately with the spin-polarized local density approximation with a small effective Hubbard parameter. The effect of increase on site coulomb repulsion at high pressure mimicked by larger U values helps to rationalize the recently observed quantum phase transition.