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Doping an antiferromagnetic insulator : A route to an antiferromagnetic metallic phase PRIYA MAHADEVAN, SHISHIR PANDEY, S.N.Bose National Centre for Basic Sciences, D.D. SARMA, SSCU, Indian Institute of Science, Bangalore — Usually antiferromagnetism is accompanied by an insulating character of the ground state, while ferromagnetism is accompanied by metallicity. In the limit of half-filling, the Hubbard model yields an antiferromagnetic insulator as the ground state. From the Nagaoka theorem we expect ferromagnetism at any finite electron doping of this half filled state. Numerical studies on the other hand, have however shown, that at low doping concentrations one has a narrow region of an antiferromagnetic metallic phase. The question is whether this is realizable in real materials. Among the 3d transition metal oxides, this antiferromagnetic metallic phase has remained elusive as strong electron-phonon coupling results in a different phase diagram. The 5d transition metal oxides are therefore more suitable. In this work we solve a multiband Hubbard model relevant for a 5d transition metal oxide within a mean-field approach and show that the large bandwidth and the small intra-atomic Hund's exchange associated with this limit gives us a robust AFM-M ground state for 25% electron doping. The conclusions are supported by ab-initio electronic structure calculations for NaOsO₃.

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