Transition Metal Oxides: Mott Transition under Pressure

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The electron-electron interaction renders many transition metal oxides under ambient conditions magnetic insulators [1]. Applied pressure leads on one hand to destruction of the local magnetic moment and on the other hand to insulator-metal transition. We study the mechanism and relationship of these two phenomena in the case of MnO, a classical strongly correlated oxide [2]. To this end we employ the approximation of dynamical mean-field theory (DMFT) [3], which allows for an accurate treatment of the local dynamical correlations. The talk will cover basic ideas of DMFT and its implementation, and numerical results for evolution of the local moments and the single-particle spectral functions of MnO and Fe_2O_3 with applied pressure will be presented.

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[3] Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).