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GW+DMFT Electronic Structure Calculations in Mott Insulators: Application to NiO NIKOLAY ZEIN, RRC "Kurchatov Institute" Moscow, SERGEY SAVRASOV, University California, Davis, GABRIEL KOTLIAR, University of Rutgers, NJ — We discuss the nature of Mott insulator ground state in transition metal oxides using newly developed GW+DMFT approach[1], which permits to join advantages of model (Hubbard-like) and density functional (LDA) calculations. The gap in LDA calculated antiferromagnetic state is usually much smaller than in experiment. Pure GW calculations increase the gap[2],but also cannot reproduce the paramagnetic insulating state. In GW+DMFT approach, without any fitting parameters, we calculate electronic structures of both antiferromagnetic and paramagnetic insulating states. We discuss relative position of d-metal and p-oxygen states,problems of renormalization of both electronic states near Fermi level and effective interaction at small energies, changes in static interaction under development of the gap in the paramagnetic state, effect of nearly filled bands on the value of self-energy correlation contribution. [1] N.E.Zein, S.Savrasov, G.Kotliar cond-mat/0511064 [2] S.V.Faleev, M.van Schilfgaarde, T.Kotani Phys.Rev.Lett. 93, 126406(2004)

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