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Pressure dependence of exchange interactions and Neel temperature in transition metal oxides JULIUS OJWANG, RONALD COHEN, LUKE SHULENBURGER, Carnegie Institution of Washington, XIANGANG WAN, Nanjing University, SERJEY SAVRASOV, UC Davis Physics Department — We perform first-principles linear response computations within LDA+U and GGA+U to systematically investigate the pressure dependence of magnetic exchange interactions for archetypal transition metal oxides (TMOs): MnO, FeO, CoO, and NiO. We obtain the Neel temperatures (T_N) using Monte Carlo simulations. We find that the magnitude of the next nearest neighbor coupling constant, J2, which dominates T_N, increases with increasing pressure, while the nearest neighbor, J1, behaves differently for the four TMOs. The variation of T_N with pressure is influenced by interplay between the nearest and next nearest neighbor exchange coupling constants. Our results are found to be in agreement in general with most experiments [1-3].

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