Pressure-driven high-spin to low-spin and orbital-selective insulator to metal transition in cubic CoO LI HUANG, XI DAI, YILIN WANG, The Institute of Physics, Chinese Academy of Sciences — We studied the magnetic and spectral properties for cubic para-magnetic phases of CoO under high pressures by using \textit{ab initio} many-body method which combining local density approximation with dynamical mean-field theory. Experimentally observed metal-insulator transition at high pressure is successfully reproduced in calculations. Our calculation predicts CoO as a Mott insulator at ambient pressure and metal at extreme high pressure. In the intermediate pressure regime, our results indicate that there is an orbital selective Mott phase with $t_{2g}$ orbitals being metallic and $e_g$ orbitals being insulating. In contrast with MnO and Fe$_2$O$_3$ ($d^5$ configuration) where metal-insulator transition is accompanied by a high-spin to low-spin transition, we found that the local moment of CoO ($d^7$ configuration) decreases gradually from 2.8 ($S = 3$ states) to 1.4 ($S = 1$ states) with increasing pressure, which is in agreement with experimental data.