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Mott physics in multi-band Hubbard model with strong spin-orbit interaction LIANG DU, LI HUANG, XI DAI, Institute of Physics, The Chinese Academy of Sciences — Spin-orbit coupling and electron correlation both play very crucial roles in the Mott physics of $4d$ and $5d$ transition-metal oxides. By studying three band Hubbard model with full Hund's rule coupling and spin-orbit coupling, we show that spin-orbit coupling intends to strongly enhance the Mott transition. By means of generalized Gutzwiller variational method and dynamical mean field (DMFT) with continuous time quantum Monte Carlo (CTQMC) as impurity solver, we obtain the complete phase diagram for this problem, which can be divided into metal, Mott insulator and band insulator phases. At mean while, we have also studied the effect of the Coulomb interaction on the strength of the spin-orbital coupling in the metallic phase. Our conclusion is that the correlation effect on the spin-orbital coupling is far beyond the mean field treatment even in the intermediate coupling regime.

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