Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Local density approximation combined with Gutzwiller method for correlated electron systems[1] XIAOYU DENG, LEI WANG, XI DAI, ZHONG FANG, The Institute of Physics, Chinese Academy of Sciences P.O. Box 603, Beijing 100190, China — We introduce in detail our newly developed *ab initio* LDA+Gutzwiller (local density approximation plus Gutzwiller) method, in which the Gutzwiller variational approach is naturally incorporated with the density functional theory (DFT) through the "Gutzwiller density functional theory (GDFT)" (which is a generalization of original Kohn-Sham formalism). This method can be used for ground state determination of electron systems ranging from weakly correlated metal to strongly correlated insulators with long-range ordering. The method is fully variational, the charge-density self-consistency can be naturally achieved, and the quantities, such as total energy, linear response, can be accurately obtained similar to LDA-type calculations. We will present some applications on typical correlated systems including d-electron systems (iron, nickel, Na_xCoO_2 and so on) and f-electron systems (delta plutonium). The obtained results using LDA+Gutzwiller are in good agreement with existing experiments.

[1]We acknowledge the support from NSF of China and the 973 program of China.

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Date submitted: 17 Nov 2009 Electronic form version 1.4