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Nature of the SDW state in FeAs-based Compounds XI DAI, ZHONG FANG, GUANGTAO WANG, GANG XU, Institute of Physics, CAS, Beijing, China — We show that the significant underestimation (about 10%) of Fe-As bond length in FeAs-based compounds by LDA is due to the strong correlation effect. By properly taking into acount the on-site correlation, we are able to reproduce experimental values (to about 1%) using self-consistent LDA+Gutzwiller method. Also we will show that the strong on-site orbital fluctuation will dramatically reduce the anti-ferromagnetic long range order in the parent compound. All these results are in good agreement with experiments.

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