

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Magnetic behaviors in Fe(Se,Te) system HONGLIANG SHI, Beijing Computational Science Research Center, BEIJING COMPUTATIONAL SCIENCE RESEARCH CENTER TEAM — The magnetic behaviors in Fe(Se,Te) system are investigated systematically by using the density functional theory. Our results show that for FeSe and FeTe in their respective ground state with different magnetic configurations, the easy axis of magnetization does not have any obvious preference. As for FeSe_{0.5}Te_{0.5}, in the collinear calculation only setting the values of magnetic moments, the ground state is in the “double stripe” magnetic phase; while the “single stripe” magnetic arrangement is found to be the ground state if the easy axis of magnetization is considered in our calculations. Our spiral calculations also successfully predict the commensurate (0.5, 0.5) ordering observed in FeSe_{0.5}Te_{0.5} system experimentally. Furthermore, two incommensurate excitations near (0.5, 0.5) are also reproduced in the spin spiral states compared with the diagram of scattering plane obtained by neutron scattering.

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Date submitted: 14 Nov 2010

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