Abstract Submitted for the MAR17 Meeting of The American Physical Society

Crystal Structure, Spin Dynamics, and Nematicity of FeSe under Pressure ZHIPING YIN, YUNDI QUAN, Department of Physics and Center for Advanced Quantum Studies, Beijing Normal University — FeSe attracts much attention in recent years due to its strong frustration to magnetic, nematic and superconducting orderings. Detailed investigation of its crystal structure, electronic structure, and magnetic excitations under pressure is important for understanding the origin and relation of the different competing orderings. In this talk, we use state-of-the-art dynamical mean field theory combined with density functional theory (DMFT+DFT) to optimize the crystal structure of FeSe under pressure and compare with available experimental measurement. We further show the evolution of its electronic structure and correlation strength with pressure which shows anomalies at intermediate pressures. Finally, we discuss the changes of the dynamical magnetic susceptibility and its connection to superconductivity and nematicity with varying pressure and interaction strength.

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Date submitted: 07 Nov 2016

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