Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Crystal and electronic structure of FeSe at high pressure and low temperature YI ZHANG, RAVHI KUMAR, Department of Physics, University of Nevada, Las Vegas, STANISLAV SINOGEIKIN, YUMING XIAO, HPCAT and Carnegie Institution of Washington, Advanced Photon Source, Argonne National Laboratory, SATHISH KUMAR, Department of Physics, University of Nevada, Las Vegas, PAUL CHOW, HPCAT and Carnegie Institution of Washington, Advanced Photon Source, Argonne National Laboratory, ANDREW CORNELIUS, CHANGFENG CHEN, Department of Physics, University of Nevada, Las Vegas —
The crystal and electronic structure of FeSe at high pressure and low temperature has been identified by density functional theory (DFT) calculations and high resolution synchrotron powder x-ray diffraction. Our results demonstrate that the HPLT phase of FeSe is orthorhombic *Pbnm*. A sluggish phase transition from *Cmma* to *Pbnm* occurs at low temperature over a large pressure range of 9 GPa to 23 GPa where both phases coexist. Our calculations suggest that the distorted *Cmma* rather than the *Pbnm* phase is responsible for the reported pressure-induced T_c enhancement in FeSe. These results establish a clear picture about structural and electronic phase transitions in FeSe at HPLT and their relationships with superconductivity.

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Date submitted: 16 Nov 2009 Electronic form version 1.4