Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Electronic correlations and topological Fermi surface transition in the iron-based chalcogenides S. SKORNYAKOV, Institute of Metal Physics, Yekaterinburg, Russia and Ural Federal Univ., Yekaterinburg, Russia, I. LEONOV, Theoretical Physics III, Center for Electronic Correlations and Magnetism, Univ. Augsburg, Germany, V.I. ANISIMOV, Institute of Metal Physics, Yekaterinburg, Russia and Ural Federal Univ., Yekaterinburg, Russia, D. VOLLHARDT, Theoretical Physics III, Center for Electronic Correlations and Magnetism, Univ. Augsburg, Germany — We present results of a theoretical investigation of the electronic structure and phase stability of paramagnetic FeSe obtained within a combination of *ab initio* methods for calculating band structure and dynamical mean-field theory. Our results reveal an entire reconstruction of the Fermi surface topology upon a moderate expansion of the lattice (Lifshitz transition), with a change of magnetic correlations from the in-plane magnetic wave vector (π, π) to $(\pi, 0)$. We attribute this behavior to a correlation-induced shift of the Van Hove singularity originating from the xy and xz/yz bands at the M-point across the Fermi level. Our results predict a structural transition of FeSe upon a ca. 10 % expansion of the lattice volume as well as a topological change of the Fermi surface of FeSe upon partial substitution Se by Te, which is accompanied with a sharp increase of the local moments. We expect that these changes are responsible for the experimentally observed increase of T_c in FeSe upon doping with Te. The microscopic origin for superconductivity in this system is then due to a Van Hove singularity close to the Fermi level. This identification may open a new route to increase T_c even further.

Sergey Skornyakov
Institute of Metal Physics, Yekaterinburg, Russia and Ural Federal Univ., Yekaterinburg, Russia

Date submitted: 05 Nov 2015 Electronic form version 1.4